

**02 INFORMATION ABOUT PRINCIPAL INVESTIGATORS/PROJECT DIRECTORS(PI/PD) and
co-PRINCIPAL INVESTIGATORS/co-PROJECT DIRECTORS**

Submit only ONE copy of this form for each PI/PD and co-PI/PD identified on the proposal. The form(s) should be attached to the original proposal as specified in GPG Section II.C.a. Submission of this information is voluntary and is not a precondition of award. This information will not be disclosed to external peer reviewers. **DO NOT INCLUDE THIS FORM WITH ANY OF THE OTHER COPIES OF YOUR PROPOSAL AS THIS MAY COMPROMISE THE CONFIDENTIALITY OF THE INFORMATION.**

PI/PD Name: Martin A Walker

Gender: Male Female
Ethnicity: (Choose one response) Hispanic or Latino Not Hispanic or Latino

Race:
(Select one or more)
 American Indian or Alaska Native
 Asian
 Black or African American
 Native Hawaiian or Other Pacific Islander
 White

Disability Status:
(Select one or more)
 Hearing Impairment
 Visual Impairment
 Mobility/Orthopedic Impairment
 Other
 None

Citizenship: (Choose one) U.S. Citizen Permanent Resident Other non-U.S. Citizen

Check here if you do not wish to provide any or all of the above information (excluding PI/PD name):

REQUIRED: Check here if you are currently serving (or have previously served) as a PI, co-PI or PD on any federally funded project

Ethnicity Definition:

Hispanic or Latino. A person of Mexican, Puerto Rican, Cuban, South or Central American, or other Spanish culture or origin, regardless of race.

Race Definitions:

American Indian or Alaska Native. A person having origins in any of the original peoples of North and South America (including Central America), and who maintains tribal affiliation or community attachment.

Asian. A person having origins in any of the original peoples of the Far East, Southeast Asia, or the Indian subcontinent including, for example, Cambodia, China, India, Japan, Korea, Malaysia, Pakistan, the Philippine Islands, Thailand, and Vietnam.

Black or African American. A person having origins in any of the black racial groups of Africa.

Native Hawaiian or Other Pacific Islander. A person having origins in any of the original peoples of Hawaii, Guam, Samoa, or other Pacific Islands.

White. A person having origins in any of the original peoples of Europe, the Middle East, or North Africa.

WHY THIS INFORMATION IS BEING REQUESTED:

The Federal Government has a continuing commitment to monitor the operation of its review and award processes to identify and address any inequities based on gender, race, ethnicity, or disability of its proposed PIs/PDs. To gather information needed for this important task, the proposer should submit a single copy of this form for each identified PI/PD with each proposal. Submission of the requested information is voluntary and will not affect the organization's eligibility for an award. However, information not submitted will seriously undermine the statistical validity, and therefore the usefulness, of information received from others. Any individual not wishing to submit some or all the information should check the box provided for this purpose. (The exceptions are the PI/PD name and the information about prior Federal support, the last question above.)

Collection of this information is authorized by the NSF Act of 1950, as amended, 42 U.S.C. 1861, et seq. Demographic data allows NSF to gauge whether our programs and other opportunities in science and technology are fairly reaching and benefiting everyone regardless of demographic category; to ensure that those in under-represented groups have the same knowledge of and access to programs and other research and educational opportunities; and to assess involvement of international investigators in work supported by NSF. The information may be disclosed to government contractors, experts, volunteers and researchers to complete assigned work; and to other government agencies in order to coordinate and assess programs. The information may be added to the Reviewer file and used to select potential candidates to serve as peer reviewers or advisory committee members. See Systems of Records, NSF-50, "Principal Investigator/Proposal File and Associated Records", 63 Federal Register 267 (January 5, 1998), and NSF-51, "Reviewer/Proposal File and Associated Records", 63 Federal Register 268 (January 5, 1998).

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PI/PD Name: Antony J Williams

Gender: Male Female
Ethnicity: (Choose one response) Hispanic or Latino Not Hispanic or Latino

Race:
(Select one or more)
 American Indian or Alaska Native
 Asian
 Black or African American
 Native Hawaiian or Other Pacific Islander
 White

Disability Status:
(Select one or more)
 Hearing Impairment
 Visual Impairment
 Mobility/Orthopedic Impairment
 Other
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Citizenship: (Choose one) U.S. Citizen Permanent Resident Other non-U.S. Citizen

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PI/PD Name: Jean-Claude Bradley

Gender: Male Female
Ethnicity: (Choose one response) Hispanic or Latino Not Hispanic or Latino

Race:
(Select one or more)
 American Indian or Alaska Native
 Asian
 Black or African American
 Native Hawaiian or Other Pacific Islander
 White

Disability Status:
(Select one or more)
 Hearing Impairment
 Visual Impairment
 Mobility/Orthopedic Impairment
 Other
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PI/PD Name: Andrew S Lang

Gender: Male Female
Ethnicity: (Choose one response) Hispanic or Latino Not Hispanic or Latino

Race:
(Select one or more)
 American Indian or Alaska Native
 Asian
 Black or African American
 Native Hawaiian or Other Pacific Islander
 White

Disability Status:
(Select one or more)
 Hearing Impairment
 Visual Impairment
 Mobility/Orthopedic Impairment
 Other
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Citizenship: (Choose one) U.S. Citizen Permanent Resident Other non-U.S. Citizen

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List of Suggested Reviewers or Reviewers Not To Include (optional)

SUGGESTED REVIEWERS:

Not Listed

REVIEWERS NOT TO INCLUDE:

Not Listed

List of Suggested Reviewers or Reviewers Not To Include (optional)

SUGGESTED REVIEWERS:

Not Listed

REVIEWERS NOT TO INCLUDE:

Not Listed

List of Suggested Reviewers or Reviewers Not To Include (optional)

SUGGESTED REVIEWERS:

Not Listed

REVIEWERS NOT TO INCLUDE:

Not Listed

COVER SHEET FOR PROPOSAL TO THE NATIONAL SCIENCE FOUNDATION

PROGRAM ANNOUNCEMENT/SOLICITATION NO./CLOSING DATE/if not in response to a program announcement/solicitation enter NSF 09-29					FOR NSF USE ONLY	
PD 06-7231			08/13/09		NSF PROPOSAL NUMBER	
FOR CONSIDERATION BY NSF ORGANIZATION UNIT(S) (Indicate the most specific unit known, i.e. program, division, etc.)					0961176	
OCI - STRATEGIC TECHNOLOGIES FOR CI						
DATE RECEIVED	NUMBER OF COPIES	DIVISION ASSIGNED	FUND CODE	DUNS# (Data Universal Numbering System)	FILE LOCATION	
08/13/2009	5	01110000 OCI	7684	152606422	08/13/2009 4:56pm	
EMPLOYER IDENTIFICATION NUMBER (EIN) OR TAXPAYER IDENTIFICATION NUMBER (TIN)		SHOW PREVIOUS AWARD NO. IF THIS IS <input type="checkbox"/> A RENEWAL <input type="checkbox"/> AN ACCOMPLISHMENT-BASED RENEWAL		IS THIS PROPOSAL BEING SUBMITTED TO ANOTHER FEDERAL AGENCY? YES <input type="checkbox"/> NO <input checked="" type="checkbox"/> IF YES, LIST ACRONYM(S)		
146013200						
NAME OF ORGANIZATION TO WHICH AWARD SHOULD BE MADE			ADDRESS OF AWARDEE ORGANIZATION, INCLUDING 9 DIGIT ZIP CODE			
SUNY College at Potsdam			SUNY College at Potsdam			
AWARDEE ORGANIZATION CODE (IF KNOWN)			Pierrepont Avenue			
0028506000			Potsdam, NY. 136762294			
NAME OF PERFORMING ORGANIZATION, IF DIFFERENT FROM ABOVE			ADDRESS OF PERFORMING ORGANIZATION, IF DIFFERENT, INCLUDING 9 DIGIT ZIP CODE			
PERFORMING ORGANIZATION CODE (IF KNOWN)						
IS AWARDEE ORGANIZATION (Check All That Apply) (See GPG II.C For Definitions)		<input type="checkbox"/> SMALL BUSINESS <input type="checkbox"/> FOR-PROFIT ORGANIZATION		<input type="checkbox"/> MINORITY BUSINESS <input type="checkbox"/> WOMAN-OWNED BUSINESS		<input type="checkbox"/> IF THIS IS A PRELIMINARY PROPOSAL THEN CHECK HERE
TITLE OF PROPOSED PROJECT Collaborative Research: An Open Online Nexus for Chemistry						
REQUESTED AMOUNT \$ 1,052,226		PROPOSED DURATION (1-60 MONTHS) 36 months		REQUESTED STARTING DATE 09/01/10		SHOW RELATED PRELIMINARY PROPOSAL NO. IF APPLICABLE
CHECK APPROPRIATE BOX(ES) IF THIS PROPOSAL INCLUDES ANY OF THE ITEMS LISTED BELOW						
<input type="checkbox"/> BEGINNING INVESTIGATOR (GPG I.G.2) <input type="checkbox"/> HUMAN SUBJECTS (GPG II.D.7) Human Subjects Assurance Number _____ Exemption Subsection _____ or IRB App. Date _____						
<input type="checkbox"/> DISCLOSURE OF LOBBYING ACTIVITIES (GPG II.C.1.e) <input type="checkbox"/> INTERNATIONAL COOPERATIVE ACTIVITIES: COUNTRY/COUNTRIES INVOLVED (GPG II.C.2.j)						
<input type="checkbox"/> PROPRIETARY & PRIVILEGED INFORMATION (GPG I.D, II.C.1.d) <input type="checkbox"/> HIGH RESOLUTION GRAPHICS/OTHER GRAPHICS WHERE EXACT COLOR REPRESENTATION IS REQUIRED FOR PROPER INTERPRETATION (GPG I.G.1)						
<input type="checkbox"/> HISTORIC PLACES (GPG II.C.2.j)						
<input type="checkbox"/> EAGER* (GPG II.D.2) <input type="checkbox"/> RAPID** (GPG II.D.1)						
<input type="checkbox"/> VERTEBRATE ANIMALS (GPG II.D.6) IACUC App. Date _____ PHS Animal Welfare Assurance Number _____						
PI/PD DEPARTMENT Chemistry			PI/PD POSTAL ADDRESS Pierrepont Avenue			
PI/PD FAX NUMBER 315-267-3170			Potsdam, NY 136762294			
			United States			
NAMES (TYPED)	High Degree	Yr of Degree	Telephone Number	Electronic Mail Address		
PI/PD NAME Martin A Walker	PhD	1998	315-267-2537	walkerma@potsdam.edu		
CO-PI/PD Antony J Williams	DPhil	1988	919-685-9300	antony.williams@chemspider.com		
CO-PI/PD						
CO-PI/PD						
CO-PI/PD						

CERTIFICATION PAGE

Certification for Authorized Organizational Representative or Individual Applicant:

By signing and submitting this proposal, the Authorized Organizational Representative or Individual Applicant is: (1) certifying that statements made herein are true and complete to the best of his/her knowledge; and (2) agreeing to accept the obligation to comply with NSF award terms and conditions if an award is made as a result of this application. Further, the applicant is hereby providing certifications regarding debarment and suspension, drug-free workplace, and lobbying activities (see below), nondiscrimination, and flood hazard insurance (when applicable) as set forth in the NSF Proposal & Award Policies & Procedures Guide, Part I: the Grant Proposal Guide (GPG) (NSF 09-29). Willful provision of false information in this application and its supporting documents or in reports required under an ensuing award is a criminal offense (U. S. Code, Title 18, Section 1001).

Conflict of Interest Certification

In addition, if the applicant institution employs more than fifty persons, by electronically signing the NSF Proposal Cover Sheet, the Authorized Organizational Representative of the applicant institution is certifying that the institution has implemented a written and enforced conflict of interest policy that is consistent with the provisions of the NSF Proposal & Award Policies & Procedures Guide, Part II, Award & Administration Guide (AAG) Chapter IV.A; that to the best of his/her knowledge, all financial disclosures required by that conflict of interest policy have been made; and that all identified conflicts of interest will have been satisfactorily managed, reduced or eliminated prior to the institution's expenditure of any funds under the award, in accordance with the institution's conflict of interest policy. Conflicts which cannot be satisfactorily managed, reduced or eliminated must be disclosed to NSF.

Drug Free Work Place Certification

By electronically signing the NSF Proposal Cover Sheet, the Authorized Organizational Representative or Individual Applicant is providing the Drug Free Work Place Certification contained in Exhibit II-3 of the Grant Proposal Guide.

Debarment and Suspension Certification

(If answer "yes", please provide explanation.)

Is the organization or its principals presently debarred, suspended, proposed for debarment, declared ineligible, or voluntarily excluded from covered transactions by any Federal department or agency?

Yes

No

By electronically signing the NSF Proposal Cover Sheet, the Authorized Organizational Representative or Individual Applicant is providing the Debarment and Suspension Certification contained in Exhibit II-4 of the Grant Proposal Guide.

Certification Regarding Lobbying

The following certification is required for an award of a Federal contract, grant, or cooperative agreement exceeding \$100,000 and for an award of a Federal loan or a commitment providing for the United States to insure or guarantee a loan exceeding \$150,000.

Certification for Contracts, Grants, Loans and Cooperative Agreements

The undersigned certifies, to the best of his or her knowledge and belief, that:

- (1) No federal appropriated funds have been paid or will be paid, by or on behalf of the undersigned, to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the awarding of any federal contract, the making of any Federal grant, the making of any Federal loan, the entering into of any cooperative agreement, and the extension, continuation, renewal, amendment, or modification of any Federal contract, grant, loan, or cooperative agreement.
- (2) If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with this Federal contract, grant, loan, or cooperative agreement, the undersigned shall complete and submit Standard Form-LLL, "Disclosure of Lobbying Activities," in accordance with its instructions.
- (3) The undersigned shall require that the language of this certification be included in the award documents for all subawards at all tiers including subcontracts, subgrants, and contracts under grants, loans, and cooperative agreements and that all subrecipients shall certify and disclose accordingly.

This certification is a material representation of fact upon which reliance was placed when this transaction was made or entered into. Submission of this certification is a prerequisite for making or entering into this transaction imposed by section 1352, Title 31, U.S. Code. Any person who fails to file the required certification shall be subject to a civil penalty of not less than \$10,000 and not more than \$100,000 for each such failure.

Certification Regarding Nondiscrimination

By electronically signing the NSF Proposal Cover Sheet, the Authorized Organizational Representative is providing the Certification Regarding Nondiscrimination contained in Exhibit II-6 of the Grant Proposal Guide.

Certification Regarding Flood Hazard Insurance

Two sections of the National Flood Insurance Act of 1968 (42 USC §4012a and §4106) bar Federal agencies from giving financial assistance for acquisition or construction purposes in any area identified by the Federal Emergency Management Agency (FEMA) as having special flood hazards unless the:

- (1) community in which that area is located participates in the national flood insurance program; and
- (2) building (and any related equipment) is covered by adequate flood insurance.

By electronically signing the NSF Proposal Cover Sheet, the Authorized Organizational Representative or Individual Applicant located in FEMA-designated special flood hazard areas is certifying that adequate flood insurance has been or will be obtained in the following situations:

- (1) for NSF grants for the construction of a building or facility, regardless of the dollar amount of the grant; and
- (2) for other NSF Grants when more than \$25,000 has been budgeted in the proposal for repair, alteration or improvement (construction) of a building or facility.

AUTHORIZED ORGANIZATIONAL REPRESENTATIVE		SIGNATURE	DATE
NAME Kathleen H Chapman		Electronic Signature	Aug 13 2009 4:53PM
TELEPHONE NUMBER 315-267-2537	ELECTRONIC MAIL ADDRESS chapmakh@potdam.edu	FAX NUMBER 315-267-3120	

* EAGER - EARly-concept Grants for Exploratory Research

** RAPID - Grants for Rapid Response Research

COVER SHEET FOR PROPOSAL TO THE NATIONAL SCIENCE FOUNDATION

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FOR CONSIDERATION BY NSF ORGANIZATION UNIT(S) (Indicate the most specific unit known, i.e. program, division, etc.)					0960987	
OCI - STRATEGIC TECHNOLOGIES FOR CI						
DATE RECEIVED	NUMBER OF COPIES	DIVISION ASSIGNED	FUND CODE	DUNS# (Data Universal Numbering System)	FILE LOCATION	
08/13/2009	5	01110000 OCI	7684	002604817	08/13/2009 4:57pm	
EMPLOYER IDENTIFICATION NUMBER (EIN) OR TAXPAYER IDENTIFICATION NUMBER (TIN)		SHOW PREVIOUS AWARD NO. IF THIS IS <input type="checkbox"/> A RENEWAL <input type="checkbox"/> AN ACCOMPLISHMENT-BASED RENEWAL		IS THIS PROPOSAL BEING SUBMITTED TO ANOTHER FEDERAL AGENCY? YES <input type="checkbox"/> NO <input checked="" type="checkbox"/> IF YES, LIST ACRONYM(S)		
231352630						
NAME OF ORGANIZATION TO WHICH AWARD SHOULD BE MADE			ADDRESS OF AWARDEE ORGANIZATION, INCLUDING 9 DIGIT ZIP CODE			
Drexel University			Drexel University			
AWARDEE ORGANIZATION CODE (IF KNOWN)			3201 Arch Street			
0032565000			Philadelphia, PA. 191042737			
NAME OF PERFORMING ORGANIZATION, IF DIFFERENT FROM ABOVE			ADDRESS OF PERFORMING ORGANIZATION, IF DIFFERENT, INCLUDING 9 DIGIT ZIP CODE			
PERFORMING ORGANIZATION CODE (IF KNOWN)						
IS AWARDEE ORGANIZATION (Check All That Apply) (See GPG II.C For Definitions) <input type="checkbox"/> SMALL BUSINESS <input type="checkbox"/> MINORITY BUSINESS <input type="checkbox"/> IF THIS IS A PRELIMINARY PROPOSAL THEN CHECK HERE <input type="checkbox"/> FOR-PROFIT ORGANIZATION <input type="checkbox"/> WOMAN-OWNED BUSINESS						
TITLE OF PROPOSED PROJECT Collaborative Research: An Open Online Nexus for Chemistry						
REQUESTED AMOUNT	PROPOSED DURATION (1-60 MONTHS)	REQUESTED STARTING DATE	SHOW RELATED PRELIMINARY PROPOSAL NO. IF APPLICABLE			
\$ 37,187	36 months	09/01/10				
CHECK APPROPRIATE BOX(ES) IF THIS PROPOSAL INCLUDES ANY OF THE ITEMS LISTED BELOW						
<input type="checkbox"/> BEGINNING INVESTIGATOR (GPG I.G.2) <input type="checkbox"/> HUMAN SUBJECTS (GPG II.D.7) Human Subjects Assurance Number _____ Exemption Subsection _____ or IRB App. Date _____						
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<input type="checkbox"/> VERTEBRATE ANIMALS (GPG II.D.6) IACUC App. Date _____ PHS Animal Welfare Assurance Number _____						
PI/PD DEPARTMENT			PI/PD POSTAL ADDRESS			
Department of Chemistry			3141 Chestnut Street			
PI/PD FAX NUMBER			Philadelphia, PA 19104			
215-895-1265			United States			
NAMES (TYPED)	High Degree	Yr of Degree	Telephone Number	Electronic Mail Address		
PI/PD NAME	Jean-Claude Bradley	PhD	1993	215-895-2647	bradlejc@drexel.edu	
CO-PI/PD						
CO-PI/PD						
CO-PI/PD						
CO-PI/PD						

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- (2) If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with this Federal contract, grant, loan, or cooperative agreement, the undersigned shall complete and submit Standard Form-LLL, "Disclosure of Lobbying Activities," in accordance with its instructions.
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- (2) for other NSF Grants when more than \$25,000 has been budgeted in the proposal for repair, alteration or improvement (construction) of a building or facility.

AUTHORIZED ORGANIZATIONAL REPRESENTATIVE		SIGNATURE	DATE
NAME Margaret Vigiolto		Electronic Signature	Aug 13 2009 10:51AM
TELEPHONE NUMBER 215-895-2311	ELECTRONIC MAIL ADDRESS vigiolto@drexel.edu	FAX NUMBER 215-895-6699	

* EAGER - EARly-concept Grants for Exploratory Research

** RAPID - Grants for Rapid Response Research

COVER SHEET FOR PROPOSAL TO THE NATIONAL SCIENCE FOUNDATION

PROGRAM ANNOUNCEMENT/SOLICITATION NO./CLOSING DATE/if not in response to a program announcement/solicitation enter NSF 09-29					FOR NSF USE ONLY	
PD 06-7231			08/13/09		NSF PROPOSAL NUMBER	
FOR CONSIDERATION BY NSF ORGANIZATION UNIT(S) (Indicate the most specific unit known, i.e. program, division, etc.)					0961175	
OCI - STRATEGIC TECHNOLOGIES FOR CI						
DATE RECEIVED	NUMBER OF COPIES	DIVISION ASSIGNED	FUND CODE	DUNS# (Data Universal Numbering System)	FILE LOCATION	
08/13/2009	5	01110000 OCI	7684	058080060	08/13/2009 4:57pm	
EMPLOYER IDENTIFICATION NUMBER (EIN) OR TAXPAYER IDENTIFICATION NUMBER (TIN)		SHOW PREVIOUS AWARD NO. IF THIS IS <input type="checkbox"/> A RENEWAL <input type="checkbox"/> AN ACCOMPLISHMENT-BASED RENEWAL		IS THIS PROPOSAL BEING SUBMITTED TO ANOTHER FEDERAL AGENCY? YES <input type="checkbox"/> NO <input checked="" type="checkbox"/> IF YES, LIST ACRONYM(S)		
730739626						
NAME OF ORGANIZATION TO WHICH AWARD SHOULD BE MADE			ADDRESS OF AWARDEE ORGANIZATION, INCLUDING 9 DIGIT ZIP CODE			
Oral Roberts University			Oral Roberts University 7777 South Lewis Tulsa, OK. 741710003			
AWARDEE ORGANIZATION CODE (IF KNOWN)						
0039859000						
NAME OF PERFORMING ORGANIZATION, IF DIFFERENT FROM ABOVE			ADDRESS OF PERFORMING ORGANIZATION, IF DIFFERENT, INCLUDING 9 DIGIT ZIP CODE			
PERFORMING ORGANIZATION CODE (IF KNOWN)						
IS AWARDEE ORGANIZATION (Check All That Apply) (See GPG II.C For Definitions)		<input type="checkbox"/> SMALL BUSINESS <input type="checkbox"/> FOR-PROFIT ORGANIZATION		<input type="checkbox"/> MINORITY BUSINESS <input type="checkbox"/> WOMAN-OWNED BUSINESS		<input type="checkbox"/> IF THIS IS A PRELIMINARY PROPOSAL THEN CHECK HERE
TITLE OF PROPOSED PROJECT Collaborative Research: An Open Online Nexus for Chemistry						
REQUESTED AMOUNT \$	PROPOSED DURATION (1-60 MONTHS)	REQUESTED STARTING DATE	SHOW RELATED PRELIMINARY PROPOSAL NO. IF APPLICABLE			
24,107	12 months	09/01/10				
CHECK APPROPRIATE BOX(ES) IF THIS PROPOSAL INCLUDES ANY OF THE ITEMS LISTED BELOW						
<input type="checkbox"/> BEGINNING INVESTIGATOR (GPG I.G.2)		<input type="checkbox"/> HUMAN SUBJECTS (GPG II.D.7) Human Subjects Assurance Number _____ Exemption Subsection _____ or IRB App. Date _____				
<input type="checkbox"/> DISCLOSURE OF LOBBYING ACTIVITIES (GPG II.C.1.e)		<input type="checkbox"/> INTERNATIONAL COOPERATIVE ACTIVITIES: COUNTRY/COUNTRIES INVOLVED (GPG II.C.2.j)				
<input type="checkbox"/> PROPRIETARY & PRIVILEGED INFORMATION (GPG I.D, II.C.1.d)						
<input type="checkbox"/> HISTORIC PLACES (GPG II.C.2.j)						
<input type="checkbox"/> EAGER* (GPG II.D.2) <input type="checkbox"/> RAPID** (GPG II.D.1)		<input type="checkbox"/> HIGH RESOLUTION GRAPHICS/OTHER GRAPHICS WHERE EXACT COLOR REPRESENTATION IS REQUIRED FOR PROPER INTERPRETATION (GPG I.G.1)				
<input type="checkbox"/> VERTEBRATE ANIMALS (GPG II.D.6) IACUC App. Date _____ PHS Animal Welfare Assurance Number _____						
PI/PD DEPARTMENT		PI/PD POSTAL ADDRESS				
Department of Mathematics		7777 South Lewis Avenue				
PI/PD FAX NUMBER		Tulsa, OK 741710003				
918-495-6660		United States				
NAMES (TYPED)	High Degree	Yr of Degree	Telephone Number	Electronic Mail Address		
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Andrew S Lang	PhD	1998	918-495-6692	alang@oru.edu		
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CO-PI/PD						
CO-PI/PD						
CO-PI/PD						

CERTIFICATION PAGE

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AUTHORIZED ORGANIZATIONAL REPRESENTATIVE		SIGNATURE	DATE
NAME Kelly Bauman		Electronic Signature	Aug 13 2009 4:52PM
TELEPHONE NUMBER 918-495-7225	ELECTRONIC MAIL ADDRESS kbauman@oru.edu	FAX NUMBER	

* EAGER - EARly-concept Grants for Exploratory Research

** RAPID - Grants for Rapid Response Research

Summary

The World Wide Web has transformed the way chemists work, and yet we are still a long way from realizing the full potential of this technology for an open network of chemical information. What is needed is some organization of resources, so as to create major hubs for the new information landscape.

It is impossible to understate the importance of the organization of information within chemistry, with more than a million new scientific articles published every year. One only needs to recall that the periodic table was born of a young professor's need to organize the material in his textbook of inorganic chemistry. Yet many of the existing information sources, such as SciFinder or Web of Science, are only really accessible to professionals working in large institutions – because of their cost – and certainly have little to offer the freshman student or the interested member of the general public.

This project aims to create a stand-alone website that is both a *repository* for chemical information in itself and also a *portal* to link to information held elsewhere. The site will function as a "wiki", a site which the users themselves can add to and modify: in this way, the site should remain relevant to the requirements and desires of its users. As the information grows, more traffic will lead to more content being added. Much of this content is unavailable from existing free websites such as Wikipedia or ChemSpider, because it lies outside the scope of those projects. The proposed nexus, or "connection/center", will deliver the full spectrum of chemical information. Research content and educational materials will be found, along with physical data, chemistry news and literature roundups. Open notebook science will be supported.

The intellectual merit in this type of project lies less in the basic idea (a wiki-based chemistry site) but more in how it is *executed*. The project will need adequate funds and staff, to achieve "critical mass." Although we cannot predict the twists and turns of future technology, we can attempt to learn from the past - to avoid the mistakes, and to learn what works well. This project brings together a group with many years of experience in presenting chemistry on the Web, through Wikipedia, ChemSpider and beyond, with the capability to develop a truly valuable and powerful chemistry wiki.

The site's openness and broad scope will naturally lead to a broad impact. It aims to serve the chemistry community in the widest sense of that term: academic and professional chemists, educators and learners of all levels, interested members of other professions and of the general public. It aims to overcome the increasing specialization of communication channels within chemistry, and to facilitate communication between chemists and with the wider community of which we all form part. Non-chemists, unfamiliar with specialized chemistry resources, will find a simple website to answer their basic questions, and wikilinks to explain jargon or technical concepts. Students from colleges and high schools will not be put off by fees or inaccessibility; a simple Web search will provide the chemical information they need to learn. High school teachers will be able to access the latest research, while downloading lesson plans and lab procedures.

In conclusion, this proposal will collect and deliver chemistry information in a completely new way. It will transform how chemists work, and it will open up chemistry to the world.

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	Total No. of Pages	Page No.* (Optional)*
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Table of Contents	1	_____
Project Description (Including Results from Prior NSF Support) (not to exceed 15 pages) (Exceed only if allowed by a specific program announcement/solicitation or if approved in advance by the appropriate NSF Assistant Director or designee)	15	_____
References Cited	3	_____
Biographical Sketches (Not to exceed 2 pages each)	6	_____
Budget (Plus up to 3 pages of budget justification)	7	_____
Current and Pending Support	3	_____
Facilities, Equipment and Other Resources	1	_____
Special Information/Supplementary Documentation	0	_____
Appendix (List below.) (Include only if allowed by a specific program announcement/ solicitation or if approved in advance by the appropriate NSF Assistant Director or designee)	_____	_____
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An Open Online Nexus for Chemistry

1. Summary

The World Wide Web has transformed the way chemists work, and yet we are still a long way from realizing the full potential of this technology for an open network of chemical information. What is needed is some organization of resources, so as to create some major hubs for the new information landscape.

It is impossible to understate the importance of the organization of information within chemistry, with more than a million new scientific articles published every year. One only needs to recall that the periodic table was born of a young professor's need to organize the material in his textbook of inorganic chemistry. Yet many of the existing information sources, such as SciFinder or Web of Science, are only really accessible to professionals working in large institutions – because of their cost – and certainly have little to offer the freshman student or the interested member of the general public.

Chemists have long recognized the intellectual merit in collecting and collating published information and repackaging it for a wider audience. The most influential journal in chemistry is not *Journal of the American Chemical Society* or *Angewandte Chemie*, it is *Chemical Reviews*. Indeed four out of the top five chemical journals (by impact factor) are review journals, which publish no original research results whatsoever.

This project aims to create a stand-alone website that is both a repository for chemical information in itself and also a portal to link to information held elsewhere. The site will function as a "wiki", a site which the users themselves can add to and modify: in this way, the site should remain relevant to the requirements and desires of its users.

The basic idea of a wiki-based chemistry site is not unusual; many such sites already exist, albeit on a small scale. With social networking being fashionable, we can expect to see many poorly thought-out wikis being created, then lying dormant. With websites, it is often the *execution* of a good idea that matters. Although we cannot predict the twists and turns of future technology, we can attempt to learn from the past - to avoid the mistakes, and to learn what works well. The difference between success and failure may lie in a few lines of code. The project brings together a group with many years of experience in presenting chemistry on the web, through Wikipedia, ChemSpider and beyond, with the capability to develop a truly valuable and powerful chemistry wiki.

The site aims to serve the chemistry community in the widest sense of that term: academic and professional chemists, educators and learners of all levels, interested members of other professions and of the general public. It aims to overcome the increasing specialization of communication channels within chemistry, and to facilitate communication between chemists and with the wider community of which we all form part.

2. Introduction

Chemists will typically search for a variety of chemical information during a normal workday. The type of information depends greatly on the specialty, but some general areas of information include:

- Chemical literature – searches for relevant papers, reviews of specific topics, current awareness, patent searching, "grey information," as well as the actual primary source material.
- Common properties of chemical compounds – structure, molecular weight, synonyms, MP, solubility.
- Chemical reaction information – synthetic pathways, reagents & catalysts, reaction conditions.
- Personal networking – job searches, other chemists working in your subject area or locality, conferences, grant advice.

- Resources – grants available, graduate programs, government support, legal & business advice.
- News and general chemical knowledge – chemical industry developments, "hot" subject areas, broad changes in law or government.

To develop a successful network hub, we must consider what works well for chemists at present. We should not create a site and then try to persuade chemists to come; rather, we should examine the current needs (and frustrations!) of chemists, then aim to meet those needs.

- Professional societies – organizations such as ACS and RSC already provide a superb array of information and resources to meet the needs of chemists, both personal and professional. These societies traditionally form the core of networks for chemists, though obviously many resources are closed to non-members. Ideally, any new information resource should be developed in collaboration with these organizations.
- Successful free information "hubs" on the Web – besides Google, chemists frequently search for chemical information on websites such as Wikipedia, ChemSpider and government sites.
- Many successful information hubs in chemistry require a fee, but they are available to some members of the chemistry community. The most powerful is Chemical Abstracts Service, which provides a remarkable array of information, particularly for searching the chemical literature. Other important resources include the Science Citation Index and Beilstein/Gmelin.
- Chemists often use information hubs that have a broader scope than just chemistry, for example the Derwent World Patents Index, Lexis-Nexis and the sites of for-profit publishers such as Elsevier (Science Direct) and Wiley.

With such great resources, why do chemists need yet another website? The recent rise of "Web 2.0" sites demonstrates the power of technologies such as wikis, and such technologies could bring great benefits to science and medicine.^[1] Unfortunately, many of the existing information networks available to chemists are closed, and many involve a fee. This approach is at odds with modern "Web 2.0" methods; as Hollett has pointed out^[2], the essential Web 2.0 attributes are "trust, openness, voluntariness and self-organization". If chemistry is to capitalize on the full power of the Internet, we need new sites that are open, and very different from websites of traditional information providers.

Younger chemists naturally turn to the Web for information, and they expect to find it there for free. A fellow-scientist recently shared his frustration that his graduate students rarely think to go beyond a Google search, to use the fee-based powerful resources that are freely available to them at the university. Rather than making a (fruitless) effort to "re-educate" every new student, we should adapt the resources to ensure that young researchers find the information they need.

Many existing open sites meet specific information needs for chemists, but there is no single site that brings together all of those needs under one "roof." ChemSpider serves as an important information hub, and includes property information on chemical compounds, spectral data, links out to the chemical literature and an entire platform for deposition and curation of data; information such as educational resources can not be found there. Other sites have narrower scope: Webreactions^[3] supplies chemical reaction listings, while ZINC^[4] provides a database of compounds for "virtual screening." The Organic Chemistry Portal^[5] describes the literature in that field, while WebElements^[6] provides award-winning descriptions of the chemical elements and their basic compounds. All are useful, yet there is no site that links all of these sites together, to allow chemists to find all their answers from one chemistry portal.

Wikipedia is defined as a general encyclopedia, and it specifically excludes original research, specialist technical documents, opinion pieces, experimental procedures, educational materials, etc. The majority of chemical information lies clearly outside the scope of Wikipedia.^[7] As such, it can never serve the broader needs of chemists, though it serves as an excellent model.

Developing an online community of chemists is the means to an end – to produce a large amount of chemistry content – it is not the purpose of the proposed site. If we can bring together even a few dozen chemists, and interest them in contributing their knowledge, we can create a paradigm-changing resource. Perhaps the most active online community at present is based at the Chemistry & Chemicals WikiProjects on Wikipedia, and this numbers around 20-50 active contributors. But this group is limited to writing encyclopedic articles. ChemSpider has a smaller group of chemists curating chemical compound/structure information. But there is no online community of chemists generating broad content to meet the wider needs of the community.

3. Objectives and significance of the proposed work

We would like to see the website serve two main purposes:

A broad repository of user-generated content

The site should allow for chemists to place information and data easily on the web, in a place where others can find it through a simple search. We envisage scientists providing a wide variety of information including experimental methods and results, topical reviews, news stories, physical data; more possibilities are given below.

Most chemistry resources (such as ACS, CAS, or even ChemSpider) currently have a "top-down" model, where the site administrators define the information needs with blank spaces. This site would instead follow a radically different approach, based on the Wikipedia model, where the contributors themselves decide what is presented and how; this should foster a culture where most contributors feel that their work is valued. It may mean that the site develops in unexpected ways, but that should be seen as an asset, not a handicap. A flourishing community of chemists of this sort will be necessary if the site is to succeed.

A free chemistry portal

We aim to provide chemists with a simple, portal through which they can find chemical information on other sites. Core content available under open licenses (for example Wikipedia articles, and perhaps some ChemSpider content) might be provided on the site itself, so that it could be integrated into the site and formatted to meet our needs. Ideally we would use on-site specific "unvandalized versions" that are periodically updated, while all editing would be redirected to the host site, in order to reduce unnecessary work and "forks". Information outside the core would ideally be provided through mashups. By having one portal that allows a standard form for structure searching (and other semantic searches) of hundreds of chemistry sites, users will not need to download dozens of different Java scripts and learn the foibles of each site separately. If our portal rises high in Google rank, as we hope, it will allow users to uncover information from small sites that may be otherwise hard to find via Google.

How to meet these objectives

In order to meet the dual goals of being both an information repository and a portal, the site should allow users to achieve either of these within a minimum of mouse-clicks, without overwhelming users with scores of buttons and search boxes. Functionality and mashups should be organized in a straightforward manner, yet they should work seamlessly around the user's needs. This means that the foundations of the site will need to be laid out carefully in advance, rather than simply being allowed to evolve in a random way. The organic nature of the site will mean that (in time) new features may just evolve; if these become a core part of the website, the main layout may need to be changed in order to remain efficient.

We assume that nearly all users will simply want to search on the site for information. These tasks need to be the most straightforward, but not to the total exclusion of others, since we want to encourage users to contribute content. Using the Wikimedia software, all pages have a text search box; the main page would also have a large area devoted to a structure drawing interface for inputting chemical structures.

All pages will have a simple URL that is "human-friendly" (e.g., the page on methanol would be called "Methanol") and which can have a permanent link. The Wikimedia software is organized in this way by default, and even older versions of pages can be seen and linked to. Such simplicity and predictability also tends to raise the Google rank of articles, helping the site to grow. Data should be organized in as many ways as possible. In particular, it must be accessible to both human users and automated scripts (machine-readability), to produce virtual databases of chemical information.

Some examples of possible content include:

- Chemical compound pages – listing physical properties, links to other sites, and if possible, prose content.
- Chemical reactions, reagents – these might link to relevant literature references
- Experimental data – physical properties, reaction results, etc. – these pages could incorporate data from open notebook science^[8] groups, and it is hoped to incorporate open notebook functionality into the site itself. Incorporating original data into the site does not only serve as a repository for such data: it also helps place that data in context for other users. In the words of the Committee on Science, Engineering, and Public Policy (COSEPUP) of the National Academies, "Unrestricted access to data used to derive conclusions also builds public confidence in the processes and outcomes of research."^[9]
- Literature reviews, summaries
- Scientific techniques
- Experimental procedures
- Educational materials – lesson plans, study problems, teaching materials, at every level from grade school to graduate school. The National Science Board has recommended the development of a "web-accessible resource of peer-evaluated STEM [Science Technology Engineering Medicine] instructional materials and best practices,"^[10] and this site could provide such a resource for the chemical sciences.
- News – the latest information on important breakthroughs, industry takeovers, government regulations, as well as site news.
- Chemistry connections – links to professional societies, blogs, scientific publishers, information on grants, conferences, etc.
- Blog – commentary on new chemistry or news
- Wikichem community – interest groups, technical help, rules & guidelines, etc.

Searching facilities are essential to be able to find the relevant content within the site. Text searching is important, but insufficient for chemical usage: the development of effective structure searching that covers all the material on the site is a key objective of this project.

What works well on the Web

The history of the Internet is littered with websites that have failed.^[11] We must learn what works well, and try to avoid the pitfalls. To be successful, we must

- Speak the language of chemists. It is vital to have any new information nexus organized by chemists for chemists.
- Know the needs of chemists. The site should provide real and relevant content, not simply trivia. It should not be centered around an exciting program, algorithm or piece of technology - that may be "cool," but is it something chemists will really use a lot? Chemists also have high professional standards; there must be systems to ensure a high level of quality.
- Use technical expertise. A website that is slow or unreliable will never flourish, even if it is tailored for chemists. Experts can also take full advantage of more advanced technology to provide additional features such as Jmol for structure displays. However, the technological wizardry should mainly lie in the background, and it should never be allowed to dominate the site.

- Have a functional layout. There is the basic requirement that users be able to find what they want with as few clicks/scrolls as possible, without being overloaded with words and boxes. Successful sites such as Amazon.com, Ebay.com and Etsy.com thrive because the site is designed around what the user wants and needs.
- Have an attractive design. Aesthetics matter! We may consider ourselves scientists who don't worry about "trivia" such eye-appeal, but in fact this can make the difference between a successful site and a failure.
- Define a clear purpose. If the site tries to do too many things, or the purpose and scope of the site is unclear, it will fail.

What works well with a wiki

With the success of Wikipedia, wikis have become popular in recent years, yet many wikis fail to achieve even a basic level of use. Since we plan to use a wiki for the main infrastructure, it is critical to organize so that it flourishes. It needs to have:

- Clear scope. Although this is important for a traditional website, it is absolutely critical for a wiki, since people will only contribute their time if they see a very clear purpose for all their hard work. Wikipedia is an encyclopedia, not a sales brochure, a "how-to" site or a site for opinion pieces. Wikitravel provides travel information, it does not try to compete with Wikipedia.
- A reason to contribute. Many wikis fail not because the purpose is poor, but because people don't care enough about helping that purpose. Wikipedia flourishes precisely because contributors have a passion for sharing their knowledge with the world, and many will work late into the night to serve that "higher purpose." Many chemists have a similar love of chemistry, but they will only share their valuable time if they can see that the site really captures that passion and adds value to their work.
- A community of users, and a community of contributors. The user community in our case is clear. But for the wiki to succeed, we also need to identify people who will contribute content to get the site off the ground. Without contributors, a wiki will completely fail.
- Critical mass. As well as needing contributors, a lot of work must be done to set up and publicize the site. Some of the early content may need to be written from scratch by paid employees, in order to build a body of content that makes the site viable.
- Scalability. Any wiki that plans to become an information nexus must be able to handle growth and traffic. Beyond the obvious technology needs, there must be a definite infrastructure to organize the contributors and direct the growth effectively. There needs to be a group of paid staff to provide commitment and continuity during times of growth - voluntary contributors come and go.
- A clear, simple set of rules. Wikipedia would have failed but for certain rules such as "neutral point of view" that have served as community norms, and helped restrict the scope of the site. Any social networking site has to deal with people as well as content, and people often have strong opinions and feelings. A certain amount of disagreement is inevitable and even good, but clear policies can help to reduce unnecessary friction. Rules should define what type of content is inappropriate or outside the scope of the site.
- A style guide. How should chemical structures be drawn? What chemical names are appropriate? Should the site use American English, British English, or both? How should pictures be formatted?
- Open access, free content. In order to allow mashups with other sites, the site must be completely open.^[2] If a wiki is not completely open to the world, it will never become significant in size, and it will not be "noticed." If a wiki charges for any significant part of its content, then nearly all volunteer contributors will be completely alienated and the site will fail. A recent report by the National Academy of Sciences also noted that "The most effective method for ensuring the integrity of research data is to ensure high standards for openness and transparency."^[12] Openness can help to provide permanence for research data, since they can be shared openly. All content needs to be clearly labeled with an open copyright; we plan to use the very successful Creative Commons license for this purpose, and follow the terms of the Berlin Declaration on Open Access to Knowledge in the

Sciences and Humanities.^[13] However, there will also be a clear set of privacy rules, to ensure that personal information is not shared publicly.

4. Suitability of proposed methods

The method chosen for achieving the objectives of the project is a public website in wiki format powered by MediaWiki software.

A wiki is a website which allows the simple creation of multiple interlinked webpages, usually through the use of software which automatically converts relatively simple text-like coding (stored as a database) into standard HTML (for display on the web). MediaWiki is a popular software package for the creation of wikis, available under a free license (GPLv2+). The reasons for these technical choices are explained below.

Choice of wiki format

Wikis are a relatively common choice of tool for the collaborative creation of documents. A wiki may be public or private: the best known example of a public wiki is the online encyclopedia Wikipedia,^[14] although the wiki-hosting company Wikia, Inc., hosts more than 10,000 public wikis on a vast range of subjects;^[15] private wikis are used by many organizations (eg, Novell, Inc.,^[16] the Royal Society of Chemistry^[17]) to prepare documents either for purely internal use or for subsequent publication in a different format. This proposal, for example, was drafted on a private wiki.

The technical requirements to contribute to a wiki document are access to the server (usually over the Internet) and a standard web browser: it is this simplicity of contribution which makes the format so popular for collaborative editing. The use of site preferences for converting the text into HTML ensures a homogenous appearance to the site. These are significant advantages over the production of multiple web pages by separate authors using more traditional HTML editors.

The use of multiple authors, and indeed the attraction of as many different contributors as possible, is an essential part of this proposal. This should enable a wide coverage of different fields with the chemical sciences, beyond the professional expertise of the PI and the workers funded under any award. More importantly, it ensures that the focus of the site remains on those areas which are most important to its users: the wiki format allows popular areas to expand with ease while still remaining integrated with the rest of the site content.

Choice of MediaWiki software

MediaWiki^[18] is the software used by the popular online encyclopedia Wikipedia and other projects of the Wikimedia Foundation, and also on the wikis hosted by Wikia, Inc., and elsewhere. It is probably the most popular wiki software,^[19] and is certainly the best known. This in itself would be a strong argument for using MediaWiki in this project, as it is the wiki software with which potential contributors are most likely to be familiar.

MediaWiki is available free of charge under the GNU General Public License 2.0 and later versions (GPLv2+).^[20] The documentation is freely available under both the GNU Free Documentation License 1.2 and later versions (GFDL1.2+)^[21] and the Creative Commons Attribution-Share Alike License version 3.0 Unported (CC-BY-SA-3.0).^[22] As such, it is classed as “free software”. It is supported by a community of several hundred volunteer developers (and at least three salaried staff members), and has proved both robust and simple to use. The latest release is version 1.15.1 (July 13, 2009).^[23]

MediaWiki functions as a database program combined with a parser to convert a text (containing simple markup) into HTML for page publication. The database contains tables for page content, internal links, users, page categorization, images and other non-text files, and other types of page: custom page types can also be created. The appearance of the site can be customized using CSS style sheets and Javascript functions are also supported. Individual users can also customize their view of the site without affecting the public view through personal CSS style sheets and Javascript functions.

In addition to the basic MediaWiki “core”, there are more than a thousand published “extensions” to MediaWiki,^[24] written (like the original program) in the PHP programming language. These extensions add optional functions to the main program: one example is cite.php, which simplifies the handling of references.^[25]

It is intended that the programming aspect of this project will concern the writing of extensions and/or Javascript functions, rather than the modification of the main MediaWiki program. All programs which are created during the project will be licensed under the GNU General Public License version 3.0^[26] and later versions, and the accompanying documentation will be licensed under both the GNU Free Documentation License version 1.3^[27] and later versions and under the Creative Commons Attribution-Share Alike License version 3.0 and later versions. This condition will be enforced contractually both for employees and for any contractors. In this way, the software resulting from this project will be freely available for reuse and modification by any other person.

Choice of creating a new website

The investigators have chosen to use the same format and basic software as the popular pre-existing website Wikipedia. However, the project concerns the development of a separate website.

The proposed website will be firmly focussed on the chemical sciences in all their forms, as opposed to the unashamed generalism of Wikipedia. The intention is to create a site “by chemists, for chemists” that will be also useful to all users of chemical information regardless of professional status or specialty. Wikipedia aims to make its articles accessible to a general audience,^[28] whereas the proposed website will allow (and encourage) more technical content where the subject matter justifies it.

The proposed website will also allow the use of functionalities which are specific to chemistry. One example is searching by chemical structure: a generalist site such as Wikipedia could never justify including structure searching as an integral part of its offer, as the proportion of chemistry searches among its usage is simply too low, but a site devoted to the chemical sciences can, indeed must, offer such a possibility.

The development of specialist content and functionality is all but impossible within the Wikipedia framework, hence the need for a new site. Chemistry is not unique in having these problems – subject-specific wikis such as PsychWiki for psychology^[29] and WikiDoc for medicine^[30] have existed for several years – but the range and complexity of chemical data present particular challenges. It is hoped that the software and content developed during this project will prove useful not only to users of the site itself but also to other sites dealing with chemical information: Wikipedia, certainly, but also other chemistry websites and private wikis.

5. Resources needed

A significant amount of support is needed to establish a major information hub of this sort. Although some websites can start very small and grow, these usually succeed by focusing on a particular niche; it is hard for such sites to have the broad scope needed to bring together diverse forms of information from all areas of chemistry. In order to succeed, our proposal requires permanent employees with a high level of expertise, working for a sustained three-year period. Salaries for these staff make up the majority of the budget. Only in this way can the site have the professional support and direction needed to succeed.

Site administrator

This person would be the figurehead of the organization, as well as guiding the overall direction and development of the site. The job description would include:

- Working with the PI and the technical developer to organize the efficient operation of the site
- Representing the organization at meetings, conferences and press briefings
- Organize the workflow of the staff in an efficient manner, and hold regular meetings
- Building connections and promoting the site within the chemical community
- Locating external data and resources that could be added to the site

- Defining the details of the layout of the site, in consultation with the technical developer, the PI, consultants, collaborators and advisers
- Building some of the initial site organization and infrastructure, and seeding with core content
- Communicating information about the site through a regular blog
- Coordinating the user community and ensuring proper copyright compliance
- Maintaining current knowledge in and around chemistry, and of the changing face of the internet

Technical developer

This person would work to add valuable technical features onto the site, organize the servers and handle bugs in the software. The job description would include:

- Leading the project developments and identifying requirements and evaluating technical options.
- Ensuring that the application achieves agreed performance and availability
- Advising on the technical requirements to deliver new technologies, products and services.
- Promoting the technical solution by attending and presenting at relevant meetings.
- Participating in general software design and development including database development; setting milestones and targets.
- Knowing state-of-the-art practices, technologies, algorithms and coding standards.
- Managing the technical aspects of the project.

Support staff

This person would perform routine office functions, including:

- Preparing letters, electronic mail, handling phone calls and routine mail/electronic mail
- Arranging meetings and taking minutes
- Receiving visitors
- Making travel arrangements and other bookings, ordering supplies.

Role of the Principal Investigator - Walker

The PI will work with the employees to guide the growth and direction of the site. Responsibilities are:

- Developing a broad vision for how the site should develop, in collaboration with the permanent staff and collaborators.
- Assisting in developing the site organization and infrastructure
- Seeding the site with core content
- Supporting the work of the site administrator - building contacts, promoting the site, etc.
- Contributing to the site blog
- Managerial oversight of employees and liaison with the services of the grantee institution for budgetary responsibility

Role of Collaborative Co-Principal Investigators - Bradley & Lang

Bradley & Lang's main work will be during the first year of the project, after which they will transition to become part of the advisory board. Responsibilities will include:

- Populating the Online Chemistry Nexus with solubility data in a database format, including temperature and mixed solvent ratios. This can be made available either live from Google Spreadsheets where the data is currently housed or via ChemSpider.
- Providing laboratory notebook pages for reporting on the details of the execution and analysis of experiments (mainly solubility measurements and Ugi reactions). In addition to including archival data, some of this work will consist of new experiments to be performed at Drexel University and ORU.
- Providing a review system for notebook pages and performing reviews to rate the content of the pages according to a list of criteria, such as:

a) reproducibility: there is sufficient detail to repeat the experiment. b) raw data acceptability: enough raw data of sufficient quality is provided and it is clear from the description when and how the data were obtained. c) analysis: the discussion and conclusions are supported by the data provided. d)

contextualization: appropriate references are cited and the place of the work within existing scholarship is made clear.

- Providing spectral data: NMR, IR and other relevant spectroscopic data accompanying experiments will be provided in the open JCAMP-DX format. This will include characterization of pure products and starting materials as well as monitoring samples and NMR spectra used to quantify solubility.
- Automated analysis of spectral data: When appropriate, such as for NMR spectra used for solubility measurements, automated analysis will be performed by bots to flag inconsistent results. For example, if extra peaks are found from the mixing of a known solute and solvent, such spectra will be flagged for manual inspection. This will require the storage of JCAMP-DX files in a database.
- The tagging and storage of reactions according to an ontology of chemical reactions, initially based on the Ugi reaction but growing as more contributors arrive.

Role of the Advisory Board and other Co-Principal Investigators

The Advisory Board will help the PI and the permanent staff with questions of strategic planning, offering "external" guidance as to what is working well (and what is working less well) on the site and as to which features should be priorities for further development. It is also hoped that individual members of the Advisory Board will be users and contributors to the site, and will help in promoting the site through their normal professional activity.

Additional support

- Support during the development phase will be provided through summer work by students (including undergraduates) and faculty. This work would provide information to "seed" the site and build the site infrastructure.
- Guidance will be provided on a day-to-day basis by the PI, and quite regularly by consultants and contractors.
- Professional legal advice will also be needed periodically.

Other facilities

A simple, appropriate domain name, *wikichem.org*, is already owned by the PI and will be used for this website. An office will be provided on the college campus for the employees to perform their work, along with the necessary furniture and computers.

6. Qualifications of the investigator and the grantee organization

The Principal Investigator has worked professionally as a chemist for 28 years, both in industry and academia. His Ph.D. in synthetic organic chemistry and his background in fine chemical processing provide him with a solid foundation in mainstream chemistry. The PI also worked in chemical information, and his Ph.D. adviser (James B. Hendrickson) helped pioneer the use of computers in chemistry. For almost five years, the PI has contributed to Wikipedia, especially in the chemistry area. He currently coordinates the Wikipedia 1.0 project, which produces offline releases and organizes article assessment.^[31]

For a project of this sort, collaboration and network-building are essential attributes. The PI recently negotiated an agreement between Chemical Abstracts Service and the Wikipedia Chemicals WikiProject whereby CAS provides Registry Number information in exchange for Wikipedia links, breaking with a long tradition of keeping such information "closed". This in turn led to the establishment of a free CAS website, providing basic chemical information for the general public.^[32] The PI's internal work on Wikipedia, such as setting up and overseeing a system for article assessment (now used on over 1.8 million articles from over 1000 projects), has required a high degree of flexibility and leadership, as will be needed for the proposed Wikichem site.

But for a project with such broad scope, a diverse group of co-PIs, senior personnel and advisers is needed. Each of these people brings a unique skill to the group. The group is as follows:

Co-PIs/Senior personnel

- Jean-Claude Bradley, organic chemistry professor at Drexel University, blogger and pioneer of Open Notebook Science.
- Elizabeth Brown, Scholarly Communications and Library Grants Officer, Binghamton Univ. Library.
- Andrew Lang, mathematics professor at Oral Roberts University in Tulsa, OK, also involved in Open Notebook Science work.
- Nigel Wheatley, a PhD chemist, former university lecturer and school teacher, now works as a science writer and consultant; an experienced Wikipedia contributor.
- Antony Williams, founder of ChemSpider, now VP Strategic Development, Royal Society of Chemistry. RSC acquired ChemSpider and continues to host it as a community resource

Advisory group

- Dirk Beetstra, Postdoctoral fellow in chemical technology at Eindhoven University of Technology; experienced Wikipedian and developer of automatic content correction tools on Wikipedia.
- Daniel Mayer, a very experienced Wikipedian with a background in biology and geology.
- Harry Pence, Distinguished Teaching Professor in chemistry at SUNY Oneonta.
- John Proetta, chemistry undergraduate, SUNY Potsdam.
- Alexander Tropsha, K.H. Lee Distinguished Professor and Chair of the School of Pharmacy at UNC-Chapel Hill, working in bioinformatics, cheminformatics, and computational drug discovery.
- Bethany Usher, professor of biological anthropology at SUNY Potsdam.
- William Wedemeyer, Assistant Professor, Dept. Biochem. & Mol. Biology, Michigan State Univ.
- Andrew Yeung, Research Assistant, Department of Chemistry, National University of Singapore; experienced Wikipedia contributor.

The grantee organization, SUNY Potsdam, is a four-year college within the State University of New York system offering a full range of subjects, including chemistry, biochemistry, geology, physics, environmental. It provides an excellent environment in which the project can flourish; the department chair of and the head of technology services have both offered their enthusiastic support (see Appendix).

7. Proposed activity

The proposed activity has been divided into three sections:

- technical activity, which requires a high-degree of programming skill and familiarity with the various software environments;
- technical-content activity, which requires a low-to-moderate degree of programming skill (or at least a collaboration with someone with some programming skills) or which requires specific expertise in the functioning of wikis;
- content activity, which requires a good general knowledge of chemistry and wiki markup, but little or no programming or other technical expertise.

As with any novel project, it is impossible to give an exact description of the activity that will be necessary or desirable. While the activity in an experimental project depends intimately on the experimental results obtained, the activity in developing the proposed site will necessarily depend on feedback from its users. The activity described here is intended to achieve the objectives described above.

Technical activity

Set up site, including choice and installation of appropriate pre-existing MediaWiki extensions

An ad hoc test site has already been set up at SUNY Potsdam. However it is expected that the installation will have to be reviewed in the light of the objectives of this proposal to ensure that it takes full advantage of the software tools which are already available for MediaWiki sites.

Extensions

A Jmol extension for MediaWiki wikis already exists, to allow display of .mol files.^[33] Hence this activity would first involve installing and testing this extension, and then modifying it if enhanced functionality and/or usability are deemed necessary.

Structure searching would initially be limited to exact structure matches. However it is hoped to extend the structure searching options to include searching by molecular fragments and reaction searching, and it is expected that development of searching options will occupy a large proportion of the technical activity of the project. There are some JavaScript structure searching tools in the Chemistry Development Kit (CDK),^[34] released under the Lesser General Public License,^[35] and the free molecule editor BKChem,^[36] written in Python, also provides a basis from which to create new free molecular structure searching tools.

Chemical markup language (CML) is a dialect of XML allowing the transfer of chemical information between different software applications.^[37] An extension is not needed to store CML files (which is trivial), but rather to integrate them with the rest of the content on the site.

Open Notebook Science is still in its infancy, and there are several approaches to its implementation. UsefulChem^[38] and the ONS Challenge^[39] are examples of ONS sites that use a wiki format to record chemical reactions and solubility measurements, respectively. Other sites effectively function using a modified blog engine^[40].

Preparation of usage statistics and regular database dumps

This point may seem trivial, but usage statistics are essential to gauge the areas of the site which attract the most interest among users, while regular database dumps (once every three months as an absolute minimum) are necessary to ensure data integrity. Database dumps will be published as compressed files for reuse, and copies will be stored away from Potsdam, New York (the location of the main servers) to insure against catastrophic server failure.

Technical-content activity

The choice of filetypes determines the types of data which can be easily stored on the site: as such, it is intended to offer as wide a range as possible, while being aware that certain proprietary filetypes are "insecure" in that they can harbor malicious code. The MediaWiki namespaces allow a top level of categorization of content: there should be sufficient distinct namespaces to allow content to be segregated by type, but not so many as to confuse users.

If content is to be reused, it must be clear under which copyright terms that reuse is possible. It is inevitable that the content hosted on the site will come under a range of different copyright licenses, not least as there are differences of opinion within the Open Science community as to which is the most appropriate copyright license to use. As such, each page of the site will have to be licensed separately, and the technical means of ensuring this put in place.

Some initial work has already been carried out at Wikipedia on the automated correction of numerical data in chemistry articles,^[41] and it is hoped to expand that work on this site. Machine-readability is essential for automated correction, but it is also useful for data mining and other forms of reuse. However, machine-readability must not be too onerous on the contributors of content, otherwise no content will be contributed. The correct trade-off between site structure and ease of contribution is essential for the success of the site.

Content activity

In MediaWiki, "Categories" are one of the main methods of organizing content (along with namespaces). Although categories can be relatively easily modified to accommodate new material, it is important to have an initial category structure in place to avoid pages "getting lost" as they are added. "Portals" are

important to new or casual users to provide an overview of the content which is available in a particular subject area. As with categories, these are "living" documents that can be easily modified but it is important to have an initial "seed structure" in place to solicit further contributions.

The site will need some initial content to attract its first users and to exemplify the possibilities for expansion. Much of this content can be adapted from Wikipedia articles, but some will have to be written *de novo*. The provision of links to other online chemistry resources is a (relatively) quick and easy way of creating useful "seed content", but these sources need to be identified and evaluated for their usefulness.

The only effective community policies are those which are developed by the community itself, but there needs to be an initial set of rules covering areas such as the scope of the site, copyright etc. It is important that these rules are as short and simple as possible: it is a recurring criticism of Wikipedia that its rules have become so involved and complex that they are a deterrent to potential contributors.

It would be naive to expect that an open site would never experience vandalism, even though it may reflect only a small proportion of changes to most public wikis, and tend to be proportional to the overall site traffic. When the community of users expands, such policing will become a community function but, at the beginning, it will probably have to be performed by the core developers. Copyright violations usually arise from misunderstanding rather than malicious intent, but again they must be removed as quickly as possible and this task will initially fall to the core developers.

8. Broad impact

The broad applicability of this project is clear in the very goals of the site - we aim to attract a wide variety of content from a wide variety of people, and create a portal that is valuable across a very wide spectrum of natural sciences. There may even be a cross-fertilization of ideas between different disciplines. A 2008 study by the Association of Research Libraries noted: "we heard anecdotal evidence that models are indeed jumping the disciplinary divide as scholars observe new models."^[42]

Range of content

This site aims to provide a service to all areas of chemistry; we hope that subprojects of people from different areas may evolve to organize content in those areas, as happens with "WikiProjects" on Wikipedia. We envisage providing - through on-site content or mashups - the complete range of chemical information, such as thermodynamic data, preparative procedures for organic chemists, nanoparticle toxicity data, inorganic chemistry reviews, etc. A significant amount of traffic is expected to come from non-chemists who use chemical techniques, or from those working in interdisciplinary areas. Internal links can help explain highly specialized technical terms, making a wiki of this sort more appealing to non-chemists. Some of our advisory group were asked to provide comments on this:

"Chemistry is at the heart of many disciplines, such as biochemistry, materials science and polymer science. The proposed nexus site would be useful to these other fields as well, amplifying the benefits for the initial investment. For illustration, undergraduate students learning biochemistry need to understand many basic chemical concepts and nomenclature, such as pKa, chirality, and relative reactivities of chemical groups. Researchers in biochemistry could also be helped by knowing the latest chemical techniques and the methods for carrying them out. Furthermore, the chemistry nexus website could be the seed from which an integrated network of such sites for related disciplines could grow."

William Wedemeyer, Assistant Professor, Dept. of Biochemistry & Mol. Biology, Michigan State Univ.

"Anthropologists and archaeologists rely on chemistry to help understand human diversity and history. For instance, chemical testing is done to determine archaeological site use, or diet composition. Anthropologists often refer to professional literature that includes chemical jargon that may not be readily understandable to them. An online database that would allow anthropologists to understand what tests are

available to help answer their research questions, and that would give them reference material to understand research literature, would be exceptionally helpful, and could encourage more collaboration between the fields."

Bethany Usher, Associate Professor, Dept. of Anthropology, SUNY Potsdam

"I am very excited about your proposal under the NSF's STCI Program to create a wiki-based hub/nexus for chemistry. As a computational medicinal chemist I work at the interface between chemistry and biology (and between chemists and biologists!). This is a very challenging position because generally speaking both groups lack necessary complimentary knowledge due to their respective training. Ultimately, both groups would like to have a drug (most often, an organic molecule) emerging from their efforts, and in this regard an access to diverse chemical information that would become available in your proposed portal would be a critical resource. The unique aspect of your proposed portal is its interactive nature with respect to its users enabling the entire community of chemists to share their knowledge and learn from the experience of others."

Alexander Tropsha, K.H. Lee Distinguished Professor and Chair of the School of Pharmacy at UNC-Chapel Hill.

One of our senior personnel provides a useful perspective - how librarians might use the site:

"Library applications for the chemical literature are almost exclusively high cost and many smaller public and academic institutions have little to no access to this type of information. Development and creation of a wiki-based hub/nexus for chemistry will provide a low-cost option for searching chemical information which is sorely needed in a time of shrinking library acquisitions budgets. Providing useful social networking tools in an interface is essential for beginning researchers. The concept and design of this wiki resource demonstrates the value and relevance of these tools in the research process."

Elizabeth Brown, Scholarly Communications and Library Grants Officer, Binghamton University Library

Different levels of knowledge and experience

Many chemistry resources are geared towards chemistry professionals, but these can be quite challenging for students and non-chemists to comprehend. Our proposed site aims to provide the information that professionals need, but this can be provide along with content written at a more basic level. A wiki is excellent at providing the *context* for information - such as linking to explanations of technical terms - without interrupting the flow of text for professional users. The lack of page limits means that content can be written at multiple levels where needed. The site is expected to prove popular among high school students and undergraduates. Our student adviser provided us with his viewpoint:

"As a senior undergraduate chemistry student, I am all too familiar with the overwhelming amount of chemical information out there. This information could range from simple physical properties to intricate reaction mechanisms of chemical synthesis. As a research chemist, I have found that the majority of my actual research time is spent searching through various sources to find the information I need. Working through a university, I have access to a number of scholarly databases which usually require a fee to view. While appreciative of this, I often find myself running into dead ends and wrong turns because there many useful databases I don't have access to. For my work, I find my key resources by skimming a huge 2500+ page chemical index, running Google searches and "Tweeting" my chemist friends across the country. My point is that the information is there but not organized in a matter which is convenient and/or effective to chemists. With an open nexus for chemistry, all of this information could be available in a coherent user-friendly manner. The demand for something like this is immense and to think how it could be used by chemists, teachers and students really blows my mind. The information which would be available could easily cut literature search times in half, leaving lots of time for chemistry in the lab. To a college chemist, this open nexus would be a blessing. I could only imagine what an impact this would have on the chemical society in years to come."

John Proetta, chemistry major/senior undergraduate, SUNY Potsdam.

Breadth of applications

The site will provide content aimed specifically at a range of groups, such as educators, students and chemistry professionals, both industrial and academic. Yet by bringing this variety of information together on one site, all of these groups have access to the full range of information resources.

The site can also contribute significantly to the infrastructure needed for *cyberlearning*, defined as "the use of networked computing and communications technologies to support learning." The vision for the Wikichem project is in close alignment with the five recommendations of the Task Force on Cyberlearning, as described in their 2008 report.^[43]

9. Why an STCI grant?

This document clearly describes a proposal for cyberinfrastructure, which is what the STCI program was created to support: "The primary purpose of the Strategic Technologies for Cyberinfrastructure Program (STCI) is to support work leading to the development and/or demonstration of innovative cyberinfrastructure services for science and engineering research"

Many current chemistry websites are small for a reason; with limited resources, they can only offer a "niche" service. If the site is to deliver good content, the scope must be narrow. A good example is Synthetic Pages,^[44] which does a very nice job of providing experimental procedures for organic chemists. However, many organic chemists may be unaware of the site, unless they stumble upon it. What is needed is something broader, but using science terms, to bring together such information in a systematic way and make it accessible - a nexus to connect sites together, a backbone of the new cyberinfrastructure.

Other related NSF programs appear to be less appropriate; the [CDI program](#) aims to "create revolutionary science and engineering research outcomes made possible by innovations and advances in computational thinking." Our proposal may lead to one or two innovations of this sort, but the core of the proposal is simply to provide existing types of information in a new way - not to generate new types of information. The project will also require some new code, but again, that is not the main purpose, making the [SHF program](#) also unsuitable.

In summary, we consider the STCI program to be perfectly aligned with our project goals.

10. Timeline

Year One

During the first year the site staff will establish the site and open it to the public. All of the major applications for the site will need a basic foundation of pages and policies. A system of quality evaluation, content moderation and (where appropriate) peer review will be set up. The core technical features of the site, such as text and structure searching, will need to be working smoothly; soon afterwards, other common features will be added, such as Jmol 3D representations. A variety of "seed" content will be uploaded, in order to attract users and (in turn) content providers. Collaborations with other chemistry content providers will be established, to allow free traffic of data through file sharing and mashups, and the necessary scripts or extensions will be put in place, to make the data available on the site promptly. As users begin to upload content, care will be taken to ensure that high standards are used from the very start, to avoid accumulation of dubious information.

Also during the first year Bradley and Lang will populate the Online Chemistry Nexus with solubility data from their own research^[45], including temperature and mixed solvent ratios. They will provide laboratory notebook pages and use these to develop a review system for notebook pages. Experimental

spectral data will be uploaded, using both characterized substances and samples from reaction monitoring and inconsistent results will be flagged via automation. They will set up a system for tagging and storing chemical reactions using an ontology.

Year Two

In year two, it is expected that the site will begin to build some momentum, and attract users in certain niche areas. The staff, researchers and advisory board will need to guide the site through this formative period, to make sure that the site develops in a desirable way. Weaknesses in the site layout or policies will need to be identified and addressed. It will become critical to promote the site in year two through regular publications and presentations. We expect that basic substructure searching will become established at this time, after a major effort by the technical developer.

Year Three

In year three, we foresee the site beginning to establish itself as a major hub of chemistry on the internet. This will bring in larger numbers of users and contributors, but there may well be "growing pains". As a community of regular user-contributors becomes established, there may well be heated debates over issues such as openness, quality and accuracy; the staff, researchers and advisory group will need to guide the community towards a fair consensus. The technical developer will continue to add new features to the site, but there may also be quite basic issues of bandwidth and server space if the site is growing rapidly. The breadth of content coverage will expand at this time into new areas, and begin to attract new users. By the end of three years, we anticipate that the site will achieve its basic aim of become a major nexus of chemists and chemical information on the internet.

11. Longevity

Three years should provide sufficient time to judge the success of this project; by the end of that time, we should know whether it has succeeded or not. However, the aim of this project is to establish a website that will endure well beyond the three year period of the funding requested here. We have considered the long term impact of the project based on three possible outcomes:

Low impact

If, for any reason, the site fails to establish itself as a major internet hub within three years, funding and support for the site may cease. However, the legacy of the site (other than basic lessons learned) could still be significant, in terms of open source chemistry applications and scripts written for use within the wiki environment. Also, much of the user-generated content may be unique, and we would work with other websites to preserve that content; it is important that such content not be lost.^[46]

Medium impact, and growing

It is possible that the site establishes itself as a valuable resource after three years, but it has not reached the point where it can support itself. In this case, we may apply for renewal of grant support from NSF, as well as seeking funding elsewhere. We would expect that this additional funding would bring the site into the "high impact, self supporting" category.

High impact, and self supporting

If the site "takes off" as intended, it should become important enough that outside organizations see value in supporting the work. This has already been seen with ChemSpider, recently acquired by the Royal Society of Chemistry.^[47] In this scenario, further NSF grant support is unlikely to be needed. The site may end up being supported by a professional body such as ACS or IUPAC, or alternatively operate as a non-profit organization like Wikipedia or the InChI Trust.^[48]

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2. The Web 2.0 way of learning with technologies. Rollett, H., Lux, M., Strohmaier, M., Dösinger, G. and Tochtermann, K., *Int. J. Learning Technology*, **2007**, 3(1), 87–107.
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4. <http://zinc.docking.org/>
5. <http://www.organic-chemistry.org/>
6. <http://www.webelements.com/>
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8. http://en.wikipedia.org/wiki/Open_Notebook_Science
9. Committee on Science, Engineering, and Public Policy (July 2009), "Ensuring the Integrity, Accessibility, and Stewardship of Research Data in the Digital Age", p. 55: http://www.nap.edu/catalog.php?record_id=12615
10. National Science Board STEM Education Recommendations for the President-Elect Obama Administration, January 11, 2009: http://www.nsf.gov/nsb/publications/2009/01_10_stem_rec_obama.pdf
11. Kent German, CNET, "[Top 10 dot-com flops](#)", accessed August 11, 2009
12. [Ensuring the Integrity, Accessibility, and Stewardship of Research Data in the Digital Age](#) Committee on Ensuring the Utility and Integrity of Research Data in a Digital Age; National Academy of Sciences, 2009. ISBN: 978-0-309-13684-6.
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14. <http://en.wikipedia.org/>
15. Source: Wikia, Inc.: http://www.wikia.com/wiki/About_Wikia
16. Eg, http://developer.novell.com/wiki/index.php/Developer_Home
17. Personal communication from Colin Bachelor, Royal Society of Chemistry.
18. <http://www.mediawiki.org/wiki/MediaWiki> . MediaWiki was developed by Magnus Manske, Brion Vibber, Lee Daniel Crocker, Tim Starling, Erik Möller, Gabriel Wicke, Ævar Arnfjörð Bjarmason, Niklas Laxström, Domas Mituzas, Rob Church, Yuri Astrakhan, Aryeh Gregor, Aaron Schulz and others: for a full list, see <http://www.mediawiki.org/wiki/Special:Code/MediaWiki/author>
19. Because of the unknown number of private wikis, it is impossible at present to determine the most popular wiki software in terms of number of sites using the software.
20. Free Software Foundation (June 1991), "GNU General Public License version 2": <http://www.gnu.org/licenses/old-licenses/gpl-2.0.txt>
21. Free Software Foundation (November 2002), "GNU Free Documentation License version 1.2": <http://www.gnu.org/licenses/old-licenses/fdl-1.2.txt>
22. Creative Commons, "Attribution-Share Alike 3.0 Unported": <http://creativecommons.org/licenses/by-sa/3.0/>
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25. Cite.php (latest version 1.11) was written by Ævar Arnfjörð Bjarmason: <http://www.mediawiki.org/wiki/Extension:Cite/Cite.php>
26. Free Software Foundation (June 2007), "GNU General Public License version 3": <http://www.gnu.org/licenses/gpl-3.0.txt>
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29. <http://www.psychwiki.com/>
30. <http://www.wikidoc.org/>
31. [Wikipedia:Version 1.0 Editorial Team](http://en.wikipedia.org/w/index.php?title=Wikipedia:Version_1.0_Editorial_Team&oldid=306575966), Wikimedia Foundation. Accessed August 13, 2009.
32. [CAS Launches Free Web-Based Resource "Common Chemistry" for General Public](http://www.cas.org/newsevents/releases/commonchemistry051209.html), CAS News Release, May 12, 2009.
33. <http://wiki.jmol.org/index.php/MediaWiki>
34. "The Chemistry Development Kit (CDK): An Open-Source Java Library for Chemo- and Bioinformatics" Steinbeck, C.; Han, Y.; Kuhn, S.; Horlacher, O.; Luttmann, E.; Willighagen, E. L. *J. Chem. Inf. Comput. Sci.* **2003**, *43*, 493–500. DOI: 10.1021/ci025584y See also http://sourceforge.net/apps/mediawiki/cdk/index.php?title=Main_Page
35. Free Software Foundation (June 2007). "Lesser General Public License version 3": <http://www.gnu.org/licenses/lgpl-3.0-standalone.html>
36. BKChem was developed by Beda Kosata: <http://bkchem.zirael.org/>
37. Further information about Chemical Markup Language, including references to peer-reviewed papers, may be found at <http://cml.sourceforge.net/>
38. <http://usefulchem.wikispaces.com/>
39. <http://onschallenge.wikispaces.com>
40. http://biolab.isis.rl.ac.uk/camerons_labblog
41. The vast majority of this work has been carried out by Dirk Beetstra: see, e.g., http://en.wikipedia.org/wiki/Wikipedia:Bots/Requests_for_approval/CheMoBot_2
42. [Current Models of Digital Scholarly Communication:] Results of an Investigation Conducted by Ithaka for the Association of Research Libraries, November 2008, Association of Research Libraries.
43. [Fostering Learning in the Networked World: The Cyberlearning Opportunity and Challenge](http://www.nsf.gov/pubs/2008/nsf08204/nsf08204.pdf), A 21st Century Agenda from the National Science Foundation, Report of the NSF Task Force on Cyberlearning, June 24, 2008, National Science Foundation.
44. <http://www.syntheticpages.org/>
45. Bradley, J.-C.; Guha, R.; Lang, A.; Lindenbaum, P.; Neylon, C.; Williams, A.J. and Willighagen, E. Beautiful Data: The Stories Behind Elegant Data Solutions, Chapter 16: Beautifying Data in the Real World, Eds: Segaran, T. and Hammerbacher, J. O'Reilly Media, 2009.

46. [Keeping the records of science accessible: can we afford it?](#). Report on the 2008 Annual Conference of the Alliance for Permanent Access, Budapest, November 4, 2008, Alliance for Permanent Access.
47. [RSC acquires ChemSpider](#), RSC Press Release, 11 May 2009.
<http://www.rsc.org/AboutUs/News/PressReleases/2009/ChemSpider.asp>
48. [Launch of the InChI Trust](#), Nature Publishing Group Press Release, 21 July 2009.
http://www.nature.com/press_releases/inchitrust.html

Biographical Sketch – Martin Alec Walker

A. Professional Preparation

University of Bristol, United Kingdom	Chemistry	B.Sc. Hons. 1981
Brandeis University, Waltham, MA	Organic Chemistry	Ph.D. 1998
National Research Council	EPR Single Crystals	1988-1990

B. Appointments

2007–present	Associate Professor of Chemistry, SUNY Potsdam
2001-2007	Assistant Professor of Chemistry, SUNY Potsdam
1999–2001	Assistant Professor of Chemistry, Johnson State College, VT
1998-1999	Visiting instructor, College of the Holy Cross, MA
1992-1993	Research Associate, polyOrganix Inc, Newburyport, MA
1981-1992	Development Chemist/Senior Chemist, Fine Organics, Seal Sands, United Kingdom.

C. Publications

Related Publications:

I have **not** published in peer-reviewed journals in this area; my expertise is in activities on Web 2.0 sites such as Wikipedia. I have contributed extensively to Wikipedia chemistry articles, and coordinate the Wikipedia 1.0 project. Some of this work has been documented in the press, for example:

"CAS Launches Free Web-Based Resource "Common Chemistry" for General Public," CAS News Release, May 12, 2009. <http://www.cas.org/newsevents/releases/commonchemistry051209.html>

"Chemical Abstracts to Check on Wikipedia," *Chemical and Engineering News*, March 17, 2008, p42-43. <http://pubs.acs.org/subscribe/journals/cen/86/i11/html/8611scic.html>

Brad Flora, "Online Native Ventures Off: Wikipedia Released on CD," *Econtent*, July 27, 2007. <http://www.econtentmag.com/Articles/ArticleReader.aspx?ArticleID=36785>

Anick Jesdanun, Associated Press, "Static Wikipedia now available on CD," MSNBC, April 24, 2007. <http://www.msnbc.msn.com/id/18292264/>

Jon Evans, "Information free-for-all," *Chemistry World*, February 24, 2006. <http://www.rsc.org/chemistryworld/News/2006/February/24020602.asp>

Other Publications:

These are some publications where I have been an author:

Walker, M. A. Martin Walker considers whether chemistry in space is the future for process chemistry." *Chemistry and Industry*, 5 April 2004, pages 16-17.

Walker, M. A. Process for the Preparation of Aryl Ketones Generating Reduced Amounts of Toxic ByProducts, US Patent No. 6,362,375, issued March 26, 2002 (assigned to College of the Holy Cross, Worcester, MA, USA).

Hendrickson, J. B.; Walker, M. A., A Two-Component Pericyclic Reaction for Synthesis of Substituted Benzofurans and Aryl-Quaternary Carbon Bonds. *Organic Letters* **2000**, 2, 2729-2731.

Hendrickson, J. B.; Walker, M. A.; Varvak, A.; Hussoin, M. S. Dehydration of epoxides to dienes using phosphonium anhydrides, *Synlett*, **1996**(6), 661.

D. Synergistic Activities

2004-present: Active on Wikipedia (username "Walkerma") in the Chemistry & Chemicals WikiProjects, where I have contributed many articles and rewrites, and also helped to organize and validate chemistry content on Wikipedia. This work has included advising ACS on use of wikis, and negotiating an agreement with Chemical Abstracts to release a collection of CAS numbers for open public use through Wikipedia. I spoke twice at the international wiki conference "Wikimania" in 2006, and I will also be giving two oral presentations at the 2009 Wikimania conference.

2005-present: Coordinator of the Wikipedia 1.0 project, which produces offline releases of Wikipedia. This work involved setting up a network of around 1300 WikiProjects, designing a quality assessment scheme for articles (now used on over 1.5 million articles on the English Wikipedia), and developing an algorithm for evaluating importance for Wikipedia articles. All of these have been used in compiling an offline selection of around 30,000 articles for release in late 2008.

http://en.wikipedia.org/wiki/Wikipedia:Version_1.0_Editorial_Team
http://en.wikipedia.org/wiki/Wikipedia:Version_1.0_Editorial_Team/Index
http://en.wikipedia.org/wiki/Wikipedia:Version_1.0_Editorial_Team/Assessment
http://en.wikipedia.org/wiki/Wikipedia:Version_1.0_Editorial_Team/SelectionBot
<http://toolserver.org/~cbm/release-data/2008-9-13/HTML/>

2004-present: Chair of the Northern New York section of the ACS until 2008, and conference chair for the 2010 Northeast Regional Meeting (NERM). This local section work involved much community outreach.

2006-present: Serving on the Advisory Boards of several online chemistry resources, including *ChemSpider*, *ARKIVOC*, *Chemistry Central Journal* and the *Journal of Cheminformatics*.

E. Collaborators and Other Affiliations

(a) Collaborations:

(2008) Deborah Knight, New York State Dept. of Environmental Conservation, Albany, NY.

(2009) Mark Noll, SUNY Brockport Department of the Earth Sciences, Brockport, NY.

(b) Ph.D. adviser:

Prof. James B. Hendrickson, Brandeis University, Waltham, MA.

Biographical Sketch – Antony John Williams

A. Professional Preparation

University of Liverpool, United Kingdom	Chemistry	B.Sc. Hons I 1985
University of London, United Kingdom	Chemistry	Ph.D. 1988
National Research Council	EPR Single Crystals	1988-1990

B. Appointments

2009-present	Vice President of Strategic Development, Royal Society of Chemistry Worldwide
2007–2009	President, ChemZoo
2007-2009	Senior Fellow, National Institute of Statistical Sciences
1997–2007	Advanced Chemistry Development Inc, Senior NMR Product Manager (1997-1999); Director of Marketing and Business Development (1999-2002); Vice president and Chief Science Officer (2002-2007)
1992-1997	NMR Technology Leader, Eastman Kodak Company, Rochester, NY
1990-1992	NMR Facility Director, University of Ottawa, Ottawa, Ontario, Canada
1988-1990	Postdoctoral Fellow, National Research Council, Ottawa, Ontario, Canada

C. Publications

Five Related Publications:

- A perspective of Publicly Accessible/Open Access Chemistry Databases, **A.J. Williams**, accepted for publication in Drug Discovery News
- M.E. Elyashberg, **A.J. Williams**, and G.E. Martin. Computer-Assisted Structure Verification and Elucidation Tools In NMR-Based Structure Elucidation. Review article. Accepted for publication in *Progress in NMR Spectroscopy* (2007)
- Beautiful Data, The Stories Behind Elegant Data Solutions, Chapter 16, Eds Toby Segaran, Jeff Hammerbacher, Series: Theory In Practice, ISBN 10: 0-596-15711-8 | ISBN 13: 9780596157111
- **A.J. Williams**, Combining Sample, Structural, and Spectral Information in an Information Management System. *Sci. Comput. Auto.* **15**, 60 (1998).
- D. E. Brown, D. McLaughlin and **A. J. Williams**. WIMS - A Web-based Information Management System. *Trends in Analytical Chemistry*, **16**, 370 (1997)

Five Other Publications:

- M. E. Elyashberg, K. A. Blinov, **A. J. Williams** and C.E. Steinbeck, The Performance Validation of Neural Network Based ¹³C NMR Prediction Using a Publicly Available Data Source. *J. Chem. Inf. Model.*, accepted for publication (2007)
- M. E. Elyashberg, K. A. Blinov, E. R. Martirosian, S. G. Molodtsov, **A. J. Williams**, and G. E. Martin, "Automated Structure Elucidation – The Benefits of a Symbiotic Relationship between the Spectroscopist and the Expert System," *J. Heterocyclic Chem.*, **40**, 1017-1029 (2003).
- **A.J. Williams**, M. S. Lee and V. Lashin, An integrated desktop mass spectrometry processing and molecular structure management system. *Spectroscopy*, **16(1)**, 38, (2001)
- **A.J. Williams**, Recent Advances in NMR Prediction and Automated Structure Elucidation Software. *Current Opinion in Drug Discovery & Development* **3**, 298 (2000)

- **A.J. Williams**, Spectroscopy management needs as part of an analytical laboratory information management system. *Spectroscopy* **14**, 38 (1999)

D. Synergistic Activities

2007-2009: I led a team of 5 software developers and coordinating a scientific advisory group of over two dozen people to produce an online free access resource for chemists. ChemSpider allows chemists access to almost 20 million chemical entities with associated properties and has been established with the intention of *Building a Structure Centric Community for Chemists*". Chemistry has long lacked the technological capabilities to a social networking environment to discuss chemistry research. ChemSpider is being developed with this intention in mind. I am actively participating in the development of Open Notebook Science supporting technologies

1997-2007: Led the ACD/Labs academic vision (<http://www.acdlabs.com/educators/>) for delivery of commercial grade software to academia at no cost. While managing over 30 individual desktop software components I worked to ensure the delivery of an industry-grade structure drawing software package. Over 1,000,000 copies of the software have been downloaded and there are over 300 academic institutions with site licenses (http://www.acdlabs.com/educators/chsk_licenses.html).

2001-2006: Participant as a member of the Division VIII Chemical Nomenclature in Organic Chemistry IUPAC committee.

E. Collaborators and Other Affiliations

(a) Collaborators and Co-authors within the last 48 months:

Dr Jean-Claude Bradley, Drexel University; Dr Kirill Blinov, ACD/Labs Moscow Inc; Dr Mikhail Elyashberg, ACD/Labs Moscow Inc.; Dr David Lankin, University of Chicago; Dr. Gary Martin, Schering-Plough; Dr Kent Mills, Pfizer; Dr. Jacqueline Hughes-Oliver, North Carolina State University; Dr John Porco, Boston University; Dr William Reynolds, University of Toronto; Dr Ann Richards, Environmental Protection Agency; Dr Gil Rishton, University of the Channel Islands; Dr. Gary Sharman, Eli Lilly; Dr. A.J. Simpson, University of Toronto; Dr. Tim Spitzer, GlaxoSmithKline; Dr Alex Tropsha, University of North Carolina; Dr. S. Stanley Young, NISS; Dr Zsolt Zsoldos, Simbiosys Inc;

(b) Graduate Advisor:

Ph.D. Advisor: Dr. Duncan Gillies, University of London, United Kingdom

Postgraduate Advisor: Keith Preston, national Research Council, Canada

Biographical Sketch - Elizabeth Anne Brown

Professional Preparation

University of Virginia	Chemistry	BA 1990
University of Pittsburgh	Chemistry	MS 1992
University of Texas, Austin	Librarianship	MLIS 1998

Appointments

1. Associate Librarian, Binghamton University, NY 2004 –date
2. Senior Assistant Librarian, Binghamton University, NY 2001 - 2004
3. Adjunct Lecturer, Harpur College, Binghamton University, NY 1999-2000
4. Assistant Librarian, Binghamton University, NY 1998 – 2001
5. Veterinary Research Assistant, New Bolton Center, University of Pennsylvania School of Veterinary Medicine, PA 1993-1996

Publications

Related Publication (Book):

Brown, Elizabeth A., *Sudden Selector's Guide to Chemistry Information Resources*, ALCTS Sudden Selectors Series, ALA Press, currently in press, expected publication in 2010.

Other Publications:

Brown, Elizabeth A., Maximiek, Sarah, Rushton, Erin E. *Coding into the Great Unknown: Analyzing Instant Messaging Session Transcripts to identify user behaviors and measure quality of service*, submitted to College & Research Libraries, June 2009.

Brown, Elizabeth A., Maximiek, Sarah, Rushton, Erin E., *Connecting to Students: Launching Instant Messaging Reference at Binghamton University*, College & Undergraduate Libraries, 13 (4): 31-42, 2006.

McManus, Alesia, Brown, Elizabeth A., Hulbert, Debbie, Maximiek, Sarah, Rushton, Erin, *Implementing E-reserves using the new Blackboard Content System*, The Journal of Interlibrary Loan, Document Delivery & E-Reserve, 16 (4) 85-92, 2005.

Synergistic Activities

1. **2006 – date:** Created programming on scholarly communications for faculty, librarian colleagues, and students. Examples include:
 - 2008 Binghamton University Provost's Multidisciplinary and Interdisciplinary Symposia, *New Approaches to Scholarly Communications and Publishing*, April 15-16, 2009
 - Co-Chair of the American Chemical Society Northeast Regional Meeting 2006 Symposia, *The Future of Scholarly Communications*, October 6, 2006
 - Speaker for the American Chemical Society Chemical Information Division Symposia *Are Chemistry Information Professionals Ready for the Future, Chemistry Librarianship: What's on the Horizon? How do we get there?*, March 23, 2009.
2. **2006 – date:** Library management of print and digital collections, including service on a variety of library administrative committees within the Binghamton University Libraries. Recent service has included the Libraries' Scholarly Communications Committee, E-Journal Preservation Task Force (2006), Collection Development and Management Steering Committee (2007 – date), and Digitization Policy Advisory Committee, (July 2008 – date). One outcome of these projects was

the creation of a Scholarly Communications website for the Binghamton University community with a suite of services to support campus scholarly and creative activity.

<http://library.lib.binghamton.edu/webdocs/scholarlycommunication.html> These projects are expected to be shared at the 2010 Special Libraries Association Annual Conference and the 2009 ACS Northeast Regional Meeting.

3. **2009 – date:** Service on two Research Libraries Group Research Information Management Support for the Research Process Program groups, Research Information Management Roadmap and Role of Libraries in Data Curation, 2009 – date. Both groups are creating documents for the library community to provide best practices for the infrastructure and services to create, share, and preserve scholarly and creative work. These reports are expected to be completed in 2010 and disseminated throughout the academic library community.
4. **2002 – date:** Presentation on the development of scientific communication skills for chemistry graduate students. A presentation at the 2005 SUNY Conference in Instructional Technology conference: Brown, Elizabeth, Jones Jr., Wayne E., *From Student to Scientist: Using a Team-Teaching Approach to Develop Scientific Communication Skills*, May 19, 2005 demonstrated a team-teaching approach to improving student learning outcomes. The course, Chemistry Graduate Seminar, was taught with Professor Wayne E. Jones, Jr. of the Department of Chemistry in 2002, 2004, and 2005.
5. **2008 – date:** Service as Chair-Elect and Chair of the Binghamton Local Section of the American Chemical Society. This position involves outreach with the local community and to local chemists.

Collaborators & Other Affiliations

Collaborator:

Professor Wayne E, Jones, Jr. Professor of Chemistry, Binghamton University

Former Advisors and Supervisors:

Professor James N. Demas, Department of Chemistry, University of Virginia

Professor Lawrence Soma, Marilyn M. Simpson Professor of Large Animal Veterinary Medicine, Department of Clinical Studies, New Bolton Center, University of Pennsylvania

Professor Kenneth C. Janda, Department of Chemistry, University of California-Irvine

Professor Emerita Julie Hallmark, School of Information, University of Texas-Austin

Jean-Claude Bradley, Drexel University

Professional Preparation

Laurentian University, Canada Chemistry B.Sc. 1989

University of Ottawa, Canada Organic Chemistry Ph.D. 1993

Appointments

2002 – Present Associate Professor of Chemistry, Drexel University

2004 – Present E-Learning Coordinator for the College of Arts and Sciences, Drexel

2007 – Present Second Life Coordinator for Drexel Island, Drexel University

1996 – 2002 Assistant Professor of Chemistry, Drexel University

1993 – 1994 Postdoctoral Researcher, Duke University

1994 – 1996 Postdoctoral Researcher, College de France

Significant Publications

1. Bradley, J.-C.; Guha, R.; Lang, A.; Lindenbaum, P.; Neylon, C.; Williams, A.J. and Willighagen, E. Beautiful Data: The Stories Behind Elegant Data Solutions, Chapter 16: Beautifying Data in the Real World, Eds: Segaran, T. and Hammerbacher, J. O'Reilly Media, 2009.

2. Bradley, J.-C.; Mirza, K. B. Osborne, T.; Williams, A.J. Owens, K. Optimization of the Ugi Reaction Using Parallel Synthesis and Automated Liquid Handling, *Journal of Visualized Experiments*, 2008 (Nov 11).

3. Bradley, J.-C. I Teach therefore iPod, *American Federation of Teachers On Campus*, February 2006, vol. 25.

4. Bradley, J.-C; McEachron, D.; Dorsey, D; Samuel, B.; Babu, S.; Boecker, J.; Haghkar, M.; Bhatt, J. The Use SMIRP for the Rapid Design and Implementation of Pedagogical Constructs: Case study of a Question-Answer-Reference Framework, *Educational Technology and Society*, 2003, 6, 1.

5. Bradley, J.C.; Samuel, B. SMIRP-A Systems Approach to Laboratory Automation, *Journal of the Association for Laboratory Automation*, 2000, 5, 48.

Synergistic Activities

1. Coordinated the purchase and construction of Drexel Island on Second Life in May 2007.

2. Created the SciFooLivesOn Conference, a presentation and poster area on Nature Island in Second Life, and organized 6 sessions in the fall of 2007 to extend discussion about the future of science from the SciFoo conference held in the summer of 2007 (<http://scifooliveson.wikispaces.com>)

3. Created the EduFrag group to enable the rapid generation of quizzes in a first-person immersive gaming environment such as Unreal Tournament or Second Life (<http://edufrag.blogspot.com>)

4. Collaborated with Andrew Lang to represent organic chemistry mechanisms and docking in Second Life.

5. Developed and coined the term Open Notebook Science, where research ideas and results are reported in real-time on blogs and wikis. The main current project involves the synthesis and testing of novel anti-malarial and anti-tumor compounds. (<http://usefulchem.wikispaces.com>)

Collaborators and Other Affiliations

Collaborators:

Rajarshi Guha (Indiana University)
David Wild (Indiana University)
Philip Rosenthal (UCSF)
Dan Zaharevitz (National Cancer Institute)
Andrew Lang (Oral Roberts University)
Yury Gogotsi (Drexel University)
Beth Ritter-Guth (Lehigh Carbon Community College)
Tsu-Soo Tan (Nanyang Institute)
Matthias Zeller (Youngstown State University)
Antony Williams (ChemSpider)
Kevin Owens (Drexel University)
Tom Osborne (Mettler-Toledo)
Cameron Neylon (University of Southampton)

Doctorate and Postdoctoral Advisors:

Tony Durst, PhD (University of Ottawa, ON, Canada)
Michael Pirrung (Duke University, Durham, NC)
Jean-Marie Lehn (College de France, Paris, France)

Collaborative Research: An Open Online Nexus for Chemistry
Oral Roberts University
Biographical Sketch – Andrew Lang

Professional Preparation

University of Kent-Canterbury, UK
Undergraduate Dissertation: Stellar Evolution and Black Holes
BSc Mathematical Physics 1991

University of Tulsa, OK
Masters Thesis: Black Holes and Singularities
MS Applied Mathematics 1993

University of Missouri
Dissertation: The Casimir Effect
PhD Mathematics 1998

Appointments

Professor of Mathematics, Oral Roberts University, 2007 – present
Honors Faculty Member, Oral Roberts University, 2002 – present
Associate Professor of Mathematics, Oral Roberts University, 2002 – 2007
Assistant Professor of Mathematics, Oral Roberts University, 1998 – 2002
Graduate Teaching Assistant, University of Missouri, 1994 – 1998
Instructor of Mathematics, University of Tulsa, 1994 (Spring Semester)
Graduate Teaching Assistant, University of Tulsa, 1992 – 1993

Publications

- ❖ **Beautifying Data in the Real World.** Jean-Claude Bradley, Rajarshi Guha, Andrew Lang, Pierre Lindenbaum, Cameron Neylon, Antony Williams, and Egon Willighagen. *Beautiful Data: The Stories Behind Elegant Data Solutions*. Toby Segaran and Jeff Hammerbacher, eds. O'Reilly Media (2009). (ISBN13: 9780596157111)
- ❖ **The Spectral Game: leveraging Open Data and crowdsourcing for education.** Jean-Claude Bradley, Robert J Lancashire, Andrew S I D Lang, and Antony J Williams, *Journal of Cheminformatics*. **1:9** (2009). (<http://www.jcheminf.com/content/1/1/9/>)
- ❖ **Visualizing Atomic Orbitals Using Second Life**, Andrew S I D Lang and David C Kobilnyk, *Journal of Virtual Worlds Research*. **1:6** (2009). (<http://journals.tdl.org/jvwr/article/view/448/465>)
- ❖ **Science & the Imagination.** Mark R Hall and Andrew S I D Lang, *National Collegiate Honors Council Archive of Honors Course Syllabi* (2008) (http://www.nchchonors.org/syllabi_sci_imagination.shtml)
- ❖ **The Language of Diversity: Restoration Toward Peace and Unity.** Mary Alice Trent, Trevor Grizzle, Andrew Lang and Elsa Rogers, eds. Cambridge Scholars Publishing (2007). (ISBN13: 9781847183828)

- ❖ **Religion, Culture, Curriculum, and Diversity in 21st Century America.** Mary Alice Trent, Trevor Grizzle, Margaret Sehorn, Andrew Lang and Elsa Rogers, eds. University Press of America (2006). (ISBN13: 9780761835585)
- ❖ **The frequency spectrum of the Casimir effect.** A S I D Lang, *Journal of Mathematical Physics*. **46**:10 (2005).
- ❖ **Modeling Basketball Free Throws.** J M Gablonsky and A S I D Lang, *SIAM REVIEW* **47**:4 (2005).
- ❖ **A Multi-Perspective Class Project at Oral Roberts University.** Andrew Lang, Aimee Raile, and Joy Thrall, *Journal of the National Collegiate Honors Council Vol. 4, No. 2.* (2003).
- ❖ **Constrained Optimization for Passive Coning Attenuator for a Spinning Spacecraft Under Thrust.** A S I D Lang and D Halsmer, *Advances in the Astronautical Sciences* V108 (2001).
- ❖ **Optimal Design of a Two-Dimensional Passive Coning Attenuator for a Spinning Spacecraft Under Thrust.** D Halsmer and A S I D Lang, *Advances in the Astronautical Sciences* V105 (2000).
- ❖ **The Electromagnetic Field Near a Dielectric Half-Space.** A D Helfer and A S I D Lang, *Journal of Physics A: Math Gen.* V32 Number 10 (1999).

Synergistic Activities

- Second Life Consultant for Nature and ACS 2007 - present
- Open Notebook Science Solubility Challenge Judge 2009 – present
- Project NExT Consultant 2008 – present
- New Faculty Mentor, Honors Program Mentor
- **Honored with** Department Faculty Member of the Year (2008), Honors Program Faculty Member of the Year (2008), University Scholar of the Year (2007), Department Faculty Member of the Year (2006), Professionalism in the Classroom Award (2000, 2003, 2008), Ralph Fagin Caught Doing Good Award (1999), Project NExT Fellowship (1999), Donald K Anderson Student Teaching Award (1998), and Gaines House Men of Engineering Outstanding Teacher Award (1998)

SUMMARY PROPOSAL BUDGET

YEAR 1

ORGANIZATION SUNY College at Potsdam				FOR NSF USE ONLY			
				PROPOSAL NO.	DURATION (months)		
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR Martin A Walker				AWARD NO.	Proposed	Granted	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)				NSF Funded Person-months		Funds Requested By proposer	Funds granted by NSF (if different)
				CAL	ACAD	SUMR	
1.	Martin A Walker - P.I.			0.00	2.00	0.00	\$ 12,869
2.	Elizabeth A Brown			0.00	0.00	0.00	0
3.	Antony J Williams			0.00	0.00	0.00	0
4.							
5.							
6.	(0) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)			0.00	0.00	0.00	0
7.	(3) TOTAL SENIOR PERSONNEL (1 - 6)			0.00	2.00	0.00	12,869
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)							
1.	(0) POST DOCTORAL SCHOLARS			0.00	0.00	0.00	0
2.	(2) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)			12.00	0.00	0.00	145,000
3.	(0) GRADUATE STUDENTS						0
4.	(2) UNDERGRADUATE STUDENTS						6,500
5.	(1) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)						20,000
6.	(0) OTHER						0
TOTAL SALARIES AND WAGES (A + B)							184,369
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)							69,694
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)							254,063
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)							
TOTAL EQUIPMENT							0
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)							5,000
2. FOREIGN							5,000
F. PARTICIPANT SUPPORT COSTS							
1.	STIPENDS	\$	0				
2.	TRAVEL		0				
3.	SUBSISTENCE		0				
4.	OTHER		0				
TOTAL NUMBER OF PARTICIPANTS (0)				TOTAL PARTICIPANT COSTS			0
G. OTHER DIRECT COSTS							
1.	MATERIALS AND SUPPLIES						23,500
2.	PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						0
3.	CONSULTANT SERVICES						10,000
4.	COMPUTER SERVICES						0
5.	SUBAWARDS						5,000
6.	OTHER						350
TOTAL OTHER DIRECT COSTS							38,850
H. TOTAL DIRECT COSTS (A THROUGH G)							302,913
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) Salary and wage base (Rate: 25.0000, Base: 184369)							
TOTAL INDIRECT COSTS (F&A)							46,092
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)							349,005
K. RESIDUAL FUNDS							0
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)							\$ 349,005
M. COST SHARING PROPOSED LEVEL \$ 0				AGREED LEVEL IF DIFFERENT \$			
PI/PD NAME Martin A Walker				FOR NSF USE ONLY			
ORG. REP. NAME* Kathleen Chapman				INDIRECT COST RATE VERIFICATION			
		Date Checked	Date Of Rate Sheet	Initials - ORG			

1 *ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET

SUMMARY PROPOSAL BUDGET

YEAR **2**

ORGANIZATION SUNY College at Potsdam				FOR NSF USE ONLY			
				PROPOSAL NO.	DURATION (months)		
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR Martin A Walker				AWARD NO.	Proposed	Granted	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)				NSF Funded Person-months		Funds Requested By proposer	Funds granted by NSF (if different)
				CAL	ACAD	SUMR	
1.	Martin A Walker - P.I.			0.00	0.00	2.00	\$ 13,255
2.	Elizabeth A Brown			0.00	0.00	0.00	0
3.	Antony J Williams - none			0.00	0.00	0.00	0
4.							
5.							
6.	(0) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)			0.00	0.00	0.00	0
7.	(3) TOTAL SENIOR PERSONNEL (1 - 6)			0.00	0.00	2.00	13,255
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)							
1.	(0) POST DOCTORAL SCHOLARS			0.00	0.00	0.00	0
2.	(2) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)			12.00	0.00	0.00	149,500
3.	(0) GRADUATE STUDENTS						0
4.	(2) UNDERGRADUATE STUDENTS						6,500
5.	(1) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)						20,600
6.	(0) OTHER						0
TOTAL SALARIES AND WAGES (A + B)							189,855
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)							73,037
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)							262,892
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)							
TOTAL EQUIPMENT							0
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)							5,000
2. FOREIGN							5,000
F. PARTICIPANT SUPPORT COSTS							
1.	STIPENDS \$ _____						0
2.	TRAVEL _____						0
3.	SUBSISTENCE _____						0
4.	OTHER _____						0
TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PARTICIPANT COSTS							0
G. OTHER DIRECT COSTS							
1.	MATERIALS AND SUPPLIES						7,500
2.	PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						0
3.	CONSULTANT SERVICES						8,000
4.	COMPUTER SERVICES						0
5.	SUBAWARDS						5,000
6.	OTHER						350
TOTAL OTHER DIRECT COSTS							20,850
H. TOTAL DIRECT COSTS (A THROUGH G)							293,742
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) Salary and wage base (Rate: 25.0000, Base: 189855)							
TOTAL INDIRECT COSTS (F&A)							47,464
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)							341,206
K. RESIDUAL FUNDS							0
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)							\$ 341,206 \$
M. COST SHARING PROPOSED LEVEL \$ 0				AGREED LEVEL IF DIFFERENT \$			
PI/PD NAME Martin A Walker				FOR NSF USE ONLY			
ORG. REP. NAME* Kathleen Chapman				INDIRECT COST RATE VERIFICATION			
		Date Checked		Date Of Rate Sheet		Initials - ORG	

2 *ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET

SUMMARY PROPOSAL BUDGET

YEAR 3

ORGANIZATION SUNY College at Potsdam				FOR NSF USE ONLY			
				PROPOSAL NO.	DURATION (months)		
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR Martin A Walker				AWARD NO.	Proposed	Granted	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)				NSF Funded Person-months		Funds Requested By proposer	Funds granted by NSF (if different)
				CAL	ACAD	SUMR	
1.	Martin A Walker - P.I.			0.00	0.00	2.00	\$ 13,653
2.	Elizabeth A Brown			0.00	0.00	0.00	0
3.	Antony J Williams - none			0.00	0.00	0.00	0
4.							
5.							
6.	(0) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)			0.00	0.00	0.00	0
7.	(3) TOTAL SENIOR PERSONNEL (1 - 6)			0.00	0.00	2.00	13,653
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)							
1.	(0) POST DOCTORAL SCHOLARS			0.00	0.00	0.00	0
2.	(2) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)			12.00	0.00	0.00	154,045
3.	(0) GRADUATE STUDENTS						0
4.	(1) UNDERGRADUATE STUDENTS						3,250
5.	(1) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)						21,218
6.	(0) OTHER						0
TOTAL SALARIES AND WAGES (A + B)							192,166
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)							75,957
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)							268,123
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)							
TOTAL EQUIPMENT							0
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)							5,000
2. FOREIGN							5,000
F. PARTICIPANT SUPPORT COSTS							
1.	STIPENDS	\$	0				
2.	TRAVEL		0				
3.	SUBSISTENCE		0				
4.	OTHER		0				
TOTAL NUMBER OF PARTICIPANTS (0)				TOTAL PARTICIPANT COSTS			0
G. OTHER DIRECT COSTS							
1.	MATERIALS AND SUPPLIES						25,500
2.	PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						0
3.	CONSULTANT SERVICES						5,000
4.	COMPUTER SERVICES						0
5.	SUBAWARDS						5,000
6.	OTHER						350
TOTAL OTHER DIRECT COSTS							35,850
H. TOTAL DIRECT COSTS (A THROUGH G)							313,973
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) Salary and wage base (Rate: 25.0000, Base: 192166)							
TOTAL INDIRECT COSTS (F&A)							48,042
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)							362,015
K. RESIDUAL FUNDS							0
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)							\$ 362,015 \$
M. COST SHARING PROPOSED LEVEL \$ 0				AGREED LEVEL IF DIFFERENT \$			
PI/PD NAME Martin A Walker				FOR NSF USE ONLY			
ORG. REP. NAME* Kathleen Chapman				INDIRECT COST RATE VERIFICATION			
		Date Checked	Date Of Rate Sheet	Initials - ORG			

3 *ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET

SUMMARY PROPOSAL BUDGET Cumulative

ORGANIZATION SUNY College at Potsdam				FOR NSF USE ONLY		
				PROPOSAL NO.	DURATION (months)	
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR Martin A Walker				AWARD NO.	Proposed	Granted
					NSF Funded Person-months	
A. SENIOR PERSONNEL: PI/PP, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)				CAL	ACAD	SUMR
1. Martin A Walker - P.I.				0.00	2.00	4.00
2. Elizabeth A Brown				0.00	0.00	0.00
3. Antony J Williams				0.00	0.00	0.00
4.						
5.						
6. () OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)				0.00	0.00	0.00
7. (3) TOTAL SENIOR PERSONNEL (1 - 6)				0.00	2.00	4.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1. (0) POST DOCTORAL SCHOLARS				0.00	0.00	0.00
2. (6) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)				36.00	0.00	0.00
3. (0) GRADUATE STUDENTS						0
4. (5) UNDERGRADUATE STUDENTS						16,250
5. (3) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)						61,818
6. (0) OTHER						0
TOTAL SALARIES AND WAGES (A + B)						566,390
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)						218,688
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)						785,078
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)						
TOTAL EQUIPMENT						0
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)						15,000
2. FOREIGN						15,000
F. PARTICIPANT SUPPORT COSTS						
1. STIPENDS \$ _____				0		
2. TRAVEL _____				0		
3. SUBSISTENCE _____				0		
4. OTHER _____				0		
TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PARTICIPANT COSTS						0
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES						56,500
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						0
3. CONSULTANT SERVICES						23,000
4. COMPUTER SERVICES						0
5. SUBAWARDS						15,000
6. OTHER						1,050
TOTAL OTHER DIRECT COSTS						95,550
H. TOTAL DIRECT COSTS (A THROUGH G)						910,628
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)						
TOTAL INDIRECT COSTS (F&A)						141,598
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)						1,052,226
K. RESIDUAL FUNDS						0
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)						\$ 1,052,226 \$
M. COST SHARING PROPOSED LEVEL \$ 0				AGREED LEVEL IF DIFFERENT \$		
PI/PP NAME Martin A Walker				FOR NSF USE ONLY		
ORG. REP. NAME* Kathleen Chapman				INDIRECT COST RATE VERIFICATION		
		Date Checked	Date Of Rate Sheet	Initials - ORG		

C *ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET

NSF Proposal: Budget Justification

The major part of the funding is to support personnel (two full-time and one part-time) for the full three year period of the grant. For a website such as this, with a very broad scope and impact, it is essential to achieve a "critical mass" and sustain that through several years; it cannot be done as a part-time project.

Antony Williams, founder of ChemSpider, has extensive technical experience in operating a major chemistry website, and he advises us that we will need to pay around \$100,000 per year in order to get the specialist technical expertise needed for the developer position. Such a person needs to be skilled in cheminformatics and database management and website administration, as well as in writing code in a variety of languages. The site administrator is also a key position, though the salary need not be as high. A third clerical/secretarial position (part-time) should ensure the smooth operation of the organization.

Clearly, the site will also need facilities and equipment. An office will be provided for the staff on campus, and this will require computers and furniture. There will need to be two servers – two are needed in case of hardware failure – and as the site grows the bandwidth and server requirements will grow also; we anticipate this occurring in year three. The servers will reside on campus, for which the IT department will receive a typical colocation fee.

The success of the site will depend on the initial content. Some of this will be imported, but the site must also be able to attract content-providers for new types of content; for this, some "seeding" of content will be needed. Much of this work will be done by the PI, co-PIs and undergraduate students.

The PI is requesting two month's salary per year for the full three years of the project. It is expected that the PI will devote a great deal of his time to establishing the site, and he plans to use a sabbatical year (in year one) for this purpose. He will work with an undergraduate to develop a user-friendly site structure containing the content needed to make the site viable. Towards the end of year one, the co-PIs Bradley and Lang will (with their student) also assist in laying the foundations of the site, focusing particularly on their specialty, open notebook science.

The site requires quite specialized expertise at the interface of chemistry and IT. Until the site is established and problems arise, it is not clear exactly who is best able to address these problems. Although simple questions will be answered through the advisory board, for complex issues we will need to use consultants or contractors. Nigel Wheatley brings a razor-sharp knowledge of chemistry combined many years of expertise from Wikipedia. Antony Williams has many years as in technical project management and cheminformatics, as well as a unique understanding of how to start with a server in the basement, and build the world's largest free chemical database.

For a website aiming for worldwide reach, travel will be an essential part of the work. Much of this will involve promoting the Wikichem initiative through presentations at scientific conferences (ACS and IUPAC meetings, etc) and expositions, and building a network of scientists who will support the site.

Start Date 9/1/10	Yr 1	Yr 2	Yr 3	Total
	10/11	11/12	12/13	
M. Walker's STCI Proposal Budget				
Salaries and Wages:				
PI - 2 mos. Yr. 1 (\$57,912 annual) - paid during AY	12869			12869
PI - 2 mos. Yr. 2 (\$59,649 annual) paid in summer		13255		13255
PI - 2 mos. Yr. 3 (\$61,439 annual) paid in summer			13653	26124
Technical Developer	95000	98000	101000	294000
Site Administrator	50000	51500	53045	15455
Office Manager/Clerical	20000	20600	21218	61818
Summer Undergraduate students (\$3,250 each)	6500	6500	3250	
Total Salaries:	184369	189855	192166	562611
Fringe Benefits:				
(Reg. salaries - 10/11 - 39%, 11/12 - 41.5%, 12/13 - 42%)	69369	70592	73610	21351
(summer only 16%)		2121	2184	4305
Undergraduate students - 5%	325	325	163	813
Total Fringes:	69694	73037	75957	21869
Travel (\$5,000 domestic, \$5,000 international)	10000	10000	10000	30000
Materials and Supplies:				
Computers	500	500	500	1500
Furniture	5000			5000
Servers and hardware	3000			3000
Server colocation	10000	2000	20000	32000
Total materials and supplies:	23500	7500	25500	56500
Consultants	10000	8000	5000	23000
Subawards	5000	5000	5000	15000

Other					
Duplicating		150	150	150	450
Telephone		150	150	150	450
Postage		50	50	50	150
Total Other:		350	350	350	1050
IDC's	(25% - reduced from federally approved rate of 73.5% of salaries and wages)	46092	47464	48042	141598
Total:		349005	341206	362015	1052226

SUMMARY PROPOSAL BUDGET

YEAR 1

ORGANIZATION Drexel University				FOR NSF USE ONLY			
				PROPOSAL NO.	DURATION (months)		
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR Jean-Claude Bradley				AWARD NO.	Proposed	Granted	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)				NSF Funded Person-months		Funds Requested By proposer	Funds granted by NSF (if different)
	CAL	ACAD	SUMR				
1. Jean-Claude Bradley - PI	0.00	0.00	1.40	\$	15,000	\$	
2.							
3.							
4.							
5.							
6. (0) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00	0.00	0.00		0		
7. (1) TOTAL SENIOR PERSONNEL (1 - 6)	0.00	0.00	1.40		15,000		
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)							
1. (0) POST DOCTORAL SCHOLARS	0.00	0.00	0.00		0		
2. (0) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	0.00	0.00	0.00		0		
3. (0) GRADUATE STUDENTS					0		
4. (2) UNDERGRADUATE STUDENTS					3,000		
5. (0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)					0		
6. (0) OTHER					0		
TOTAL SALARIES AND WAGES (A + B)					18,000		
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					4,830		
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)					22,830		
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)							
TOTAL EQUIPMENT					0		
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)					0		
2. FOREIGN					0		
F. PARTICIPANT SUPPORT COSTS							
1. STIPENDS \$ _____					0		
2. TRAVEL _____					0		
3. SUBSISTENCE _____					0		
4. OTHER _____					0		
TOTAL NUMBER OF PARTICIPANTS (0)				TOTAL PARTICIPANT COSTS	0		
G. OTHER DIRECT COSTS							
1. MATERIALS AND SUPPLIES					3,000		
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					0		
3. CONSULTANT SERVICES					0		
4. COMPUTER SERVICES					0		
5. SUBAWARDS					0		
6. OTHER					0		
TOTAL OTHER DIRECT COSTS					3,000		
H. TOTAL DIRECT COSTS (A THROUGH G)					25,830		
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) salaries and fringe (Rate: 54.0830, Base: 22830) (Cont. on Comments Page)							
TOTAL INDIRECT COSTS (F&A)					13,969		
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)					39,799		
K. RESIDUAL FUNDS					0		
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				\$	39,799	\$	
M. COST SHARING PROPOSED LEVEL \$ 0				AGREED LEVEL IF DIFFERENT \$			
PI/PD NAME Jean-Claude Bradley				FOR NSF USE ONLY			
ORG. REP. NAME* Margaret Vigiolto				INDIRECT COST RATE VERIFICATION			
		Date Checked	Date Of Rate Sheet	Initials - ORG			

1 *ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET

SUMMARY PROPOSAL BUDGET COMMENTS - Year 1

**** I- Indirect Costs
supplies (Rate: 54.0830, Base 3000)**

SUMMARY PROPOSAL BUDGET

YEAR **2**

ORGANIZATION Drexel University				FOR NSF USE ONLY			
				PROPOSAL NO.	DURATION (months)		
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR Jean-Claude Bradley				AWARD NO.	Proposed	Granted	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)				NSF Funded Person-months		Funds Requested By proposer	Funds granted by NSF (if different)
				CAL	ACAD	SUMR	
1. Jean-Claude Bradley - none				0.00	0.00	0.00	\$ 0 \$
2.							
3.							
4.							
5.							
6. (0) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)				0.00	0.00	0.00	0
7. (1) TOTAL SENIOR PERSONNEL (1 - 6)				0.00	0.00	0.00	0
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)							
1. () POST DOCTORAL SCHOLARS							
2. () OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)							
3. () GRADUATE STUDENTS							
4. () UNDERGRADUATE STUDENTS							
5. () SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)							
6. () OTHER							
TOTAL SALARIES AND WAGES (A + B)							0
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)							
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)							0
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)							
TOTAL EQUIPMENT							0
E. TRAVEL							
1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)							
2. FOREIGN							
F. PARTICIPANT SUPPORT COSTS							
1. STIPENDS \$ _____							
2. TRAVEL _____							
3. SUBSISTENCE _____							
4. OTHER _____							
TOTAL NUMBER OF PARTICIPANTS ()							
TOTAL PARTICIPANT COSTS							0
G. OTHER DIRECT COSTS							
1. MATERIALS AND SUPPLIES							
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION							
3. CONSULTANT SERVICES							
4. COMPUTER SERVICES							
5. SUBAWARDS							
6. OTHER							
TOTAL OTHER DIRECT COSTS							0
H. TOTAL DIRECT COSTS (A THROUGH G)							0
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) (Rate: , Base:)							
TOTAL INDIRECT COSTS (F&A)							0
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)							0
K. RESIDUAL FUNDS							
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)							\$ 0 \$
M. COST SHARING PROPOSED LEVEL \$				AGREED LEVEL IF DIFFERENT \$			
PI/PD NAME Jean-Claude Bradley				FOR NSF USE ONLY			
ORG. REP. NAME* Margaret Vigiolto				INDIRECT COST RATE VERIFICATION			
				Date Checked	Date Of Rate Sheet	Initials - ORG	

2 *ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET

SUMMARY PROPOSAL BUDGET

YEAR 3

ORGANIZATION Drexel University				FOR NSF USE ONLY		
				PROPOSAL NO.	DURATION (months)	
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR Jean-Claude Bradley				AWARD NO.	Proposed	Granted
					NSF Funded Person-months	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)				CAL	ACAD	SUMR
1. Jean-Claude Bradley - none				0.00	0.00	0.00
2.						
3.						
4.						
5.						
6. (0) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)				0.00	0.00	0.00
7. (1) TOTAL SENIOR PERSONNEL (1 - 6)				0.00	0.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1. () POST DOCTORAL SCHOLARS						
2. () OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)						
3. () GRADUATE STUDENTS						
4. () UNDERGRADUATE STUDENTS						
5. () SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)						
6. () OTHER						
TOTAL SALARIES AND WAGES (A + B)						0
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)						
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)						0
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)						
TOTAL EQUIPMENT						0
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)						
2. FOREIGN						
F. PARTICIPANT SUPPORT COSTS						
1. STIPENDS \$ _____						
2. TRAVEL _____						
3. SUBSISTENCE _____						
4. OTHER _____						
TOTAL NUMBER OF PARTICIPANTS () TOTAL PARTICIPANT COSTS						0
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES						
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						
3. CONSULTANT SERVICES						
4. COMPUTER SERVICES						
5. SUBAWARDS						
6. OTHER						
TOTAL OTHER DIRECT COSTS						0
H. TOTAL DIRECT COSTS (A THROUGH G)						0
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) (Rate: , Base:)						
TOTAL INDIRECT COSTS (F&A)						0
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)						0
K. RESIDUAL FUNDS						
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)						0
M. COST SHARING PROPOSED LEVEL \$				AGREED LEVEL IF DIFFERENT \$		
PI/PD NAME Jean-Claude Bradley				FOR NSF USE ONLY INDIRECT COST RATE VERIFICATION		
ORG. REP. NAME* Margaret Vigiolto						
		Date Checked	Date Of Rate Sheet	Initials - ORG		

3 *ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET

SUMMARY PROPOSAL BUDGET Cumulative

ORGANIZATION Drexel University				FOR NSF USE ONLY			
				PROPOSAL NO.	DURATION (months)		
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR Jean-Claude Bradley				AWARD NO.	Proposed	Granted	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)				NSF Funded Person-months		Funds Requested By proposer	Funds granted by NSF (if different)
				CAL	ACAD	SUMR	
1. Jean-Claude Bradley - none				0.00	0.00	1.40	\$ 15,000 \$
2.							
3.							
4.							
5.							
6. () OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)				0.00	0.00	0.00	0
7. (1) TOTAL SENIOR PERSONNEL (1 - 6)				0.00	0.00	1.40	15,000
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)							
1. (0) POST DOCTORAL SCHOLARS				0.00	0.00	0.00	0
2. (0) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)				0.00	0.00	0.00	0
3. (0) GRADUATE STUDENTS							0
4. (2) UNDERGRADUATE STUDENTS							3,000
5. (0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)							0
6. (0) OTHER							0
TOTAL SALARIES AND WAGES (A + B)							18,000
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)							4,830
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)							22,830
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)							
TOTAL EQUIPMENT							0
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)							0
2. FOREIGN							0
F. PARTICIPANT SUPPORT COSTS							
1. STIPENDS \$ _____ 0							
2. TRAVEL _____ 0							
3. SUBSISTENCE _____ 0							
4. OTHER _____ 0							
TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PARTICIPANT COSTS							0
G. OTHER DIRECT COSTS							
1. MATERIALS AND SUPPLIES							3,000
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION							0
3. CONSULTANT SERVICES							0
4. COMPUTER SERVICES							0
5. SUBAWARDS							0
6. OTHER							0
TOTAL OTHER DIRECT COSTS							3,000
H. TOTAL DIRECT COSTS (A THROUGH G)							25,830
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)							
TOTAL INDIRECT COSTS (F&A)							13,969
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)							39,799
K. RESIDUAL FUNDS							0
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)							\$ 39,799 \$
M. COST SHARING PROPOSED LEVEL \$ 0				AGREED LEVEL IF DIFFERENT \$			
PI/PD NAME Jean-Claude Bradley				FOR NSF USE ONLY			
ORG. REP. NAME* Margaret Vigiolto				INDIRECT COST RATE VERIFICATION			
		Date Checked		Date Of Rate Sheet		Initials - ORG	

C *ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET

Budget Justification Page

Summer salary (1.4 months) for the PI, support for 2 undergraduate students (\$3000) and chemicals and supplies (\$3000) is requested for the work to be done at Drexel University. Only funding for the first year is requested since the project's timeline includes seeding with content from Drexel near the end of the first year.

SUMMARY PROPOSAL BUDGET

YEAR 1

ORGANIZATION Oral Roberts University				FOR NSF USE ONLY			
				PROPOSAL NO.	DURATION (months)		
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR Andrew S Lang				AWARD NO.	Proposed	Granted	
				A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)			
				CAL	ACAD	SUMR	
1.	Andrew S Lang - Dr.			2.00	0.00	0.00	\$ 14,963
2.							
3.							
4.							
5.							
6.	(0) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)			0.00	0.00	0.00	0
7.	(1) TOTAL SENIOR PERSONNEL (1 - 6)			2.00	0.00	0.00	14,963
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)							
1.	(0) POST DOCTORAL SCHOLARS			0.00	0.00	0.00	0
2.	(0) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)			0.00	0.00	0.00	0
3.	(0) GRADUATE STUDENTS						0
4.	(0) UNDERGRADUATE STUDENTS						0
5.	(0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)						0
6.	(0) OTHER						0
TOTAL SALARIES AND WAGES (A + B)							14,963
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)							4,169
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)							19,132
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)							
TOTAL EQUIPMENT							0
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)							0
2. FOREIGN							0
F. PARTICIPANT SUPPORT COSTS							
1.	STIPENDS \$ _____						0
2.	TRAVEL _____						0
3.	SUBSISTENCE _____						0
4.	OTHER _____						0
TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PARTICIPANT COSTS							0
G. OTHER DIRECT COSTS							
1. MATERIALS AND SUPPLIES							37
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION							0
3. CONSULTANT SERVICES							0
4. COMPUTER SERVICES							0
5. SUBAWARDS							0
6. OTHER							0
TOTAL OTHER DIRECT COSTS							37
H. TOTAL DIRECT COSTS (A THROUGH G)							19,169
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) Indirect Costs Excluding Fringe (Rate: 35.0000, Base: 14963)							
TOTAL INDIRECT COSTS (F&A)							5,237
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)							24,406
K. RESIDUAL FUNDS							0
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)							\$ 24,406 \$
M. COST SHARING PROPOSED LEVEL \$ 0 AGREED LEVEL IF DIFFERENT \$							
PI/PD NAME Andrew S Lang				FOR NSF USE ONLY			
ORG. REP. NAME* Kelly Bauman				INDIRECT COST RATE VERIFICATION			
		Date Checked	Date Of Rate Sheet			Initials - ORG	

1 *ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET

SUMMARY PROPOSAL BUDGET Cumulative

ORGANIZATION Oral Roberts University				FOR NSF USE ONLY			
				PROPOSAL NO.	DURATION (months)		
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR Andrew S Lang				AWARD NO.	Proposed	Granted	
A. SENIOR PERSONNEL: PI/PI, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)				NSF Funded Person-months		Funds Requested By proposer	Funds granted by NSF (if different)
		CAL	ACAD	SUMR			
1.	Andrew S Lang - Dr.	2.00	0.00	0.00	\$	14,963	\$
2.							
3.							
4.							
5.							
6.	() OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00	0.00	0.00		0	
7.	(1) TOTAL SENIOR PERSONNEL (1 - 6)	2.00	0.00	0.00		14,963	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)							
1.	(0) POST DOCTORAL SCHOLARS	0.00	0.00	0.00		0	
2.	(0) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	0.00	0.00	0.00		0	
3.	(0) GRADUATE STUDENTS					0	
4.	(0) UNDERGRADUATE STUDENTS					0	
5.	(0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)					0	
6.	(0) OTHER					0	
TOTAL SALARIES AND WAGES (A + B)						14,963	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)						4,169	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)						19,132	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)							
TOTAL EQUIPMENT						0	
E. TRAVEL						0	
1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)						0	
2. FOREIGN						0	
F. PARTICIPANT SUPPORT COSTS							
1.	STIPENDS \$ _____					0	
2.	TRAVEL _____					0	
3.	SUBSISTENCE _____					0	
4.	OTHER _____					0	
TOTAL NUMBER OF PARTICIPANTS (0)				TOTAL PARTICIPANT COSTS		0	
G. OTHER DIRECT COSTS							
1. MATERIALS AND SUPPLIES						37	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						0	
3. CONSULTANT SERVICES						0	
4. COMPUTER SERVICES						0	
5. SUBAWARDS						0	
6. OTHER						0	
TOTAL OTHER DIRECT COSTS						37	
H. TOTAL DIRECT COSTS (A THROUGH G)						19,169	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)							
TOTAL INDIRECT COSTS (F&A)						5,237	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)						24,406	
K. RESIDUAL FUNDS						0	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)						\$ 24,406	\$
M. COST SHARING PROPOSED LEVEL \$ 0				AGREED LEVEL IF DIFFERENT \$			
PI/PI NAME Andrew S Lang				FOR NSF USE ONLY			
ORG. REP. NAME* Kelly Bauman				INDIRECT COST RATE VERIFICATION			
		Date Checked	Date Of Rate Sheet		Initials - ORG		

C *ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET

Budget Justification – Andrew Lang

Introduction

This proposal requests \$24,406 over one year.

Year 1

I have requested a summer salary of \$14,963 (2 months) of \$67,334.40 my regular academic salary (accounting for an annual 5% increase).

Fringe benefits consists of \$4,169 are calculated as 27.86% of the PI salary.

I have requested \$37 in supplies for the project.

Oral Roberts University currently does not have a federally negotiated indirect cost rate. The stated rate of 35% of salaries and wages (excluding fringe benefits) is the most recent estimated rate.

Current and Pending Support

(See GPG Section II.C.2.h for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Martin Walker	Other agencies (including NSF) to which this proposal has been/will be submitted.
Support: <input checked="" type="checkbox"/> Current <input type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support Project/Proposal Title: Development of Pollution Prevention Learning Modules within a Standards-Based Curriculum	
Source of Support: Rochester Institute of Technology Total Award Amount: \$ 14,157 Total Award Period Covered: 06/01/09 - 02/28/10 Location of Project: SUNY Potsdam Person-Months Per Year Committed to the Project. Cal:0.00 Acad: 0.00 Sumr: 2.00	
Support: <input type="checkbox"/> Current <input checked="" type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support Project/Proposal Title: Collaborative Research: An Open Online Nexus for Chemistry	
Source of Support: National Science Foundation Total Award Amount: \$ 1,052,226 Total Award Period Covered: 09/01/10 - 08/31/13 Location of Project: SUNY Potsdam Person-Months Per Year Committed to the Project. Cal:0.00 Acad: 0.00 Sumr: 2.00	
Support: <input type="checkbox"/> Current <input type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support Project/Proposal Title:	
Source of Support: Total Award Amount: \$ Total Award Period Covered: Location of Project: Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:	
Support: <input type="checkbox"/> Current <input type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support Project/Proposal Title:	
Source of Support: Total Award Amount: \$ Total Award Period Covered: Location of Project: Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:	
Support: <input type="checkbox"/> Current <input type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support Project/Proposal Title:	
Source of Support: Total Award Amount: \$ Total Award Period Covered: Location of Project: Person-Months Per Year Committed to the Project. Cal: Acad: Summ:	

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Current and Pending Support

(See GPG Section II.C.2.h for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.			
Investigator: Elizabeth Brown	Other agencies (including NSF) to which this proposal has been/will be submitted.		
Support: <input type="checkbox"/> Current <input checked="" type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support Project/Proposal Title: Collaborative Research: An Open Online Nexus for Chemistry			
Source of Support: National Science Foundation Total Award Amount: \$ 1,052,226 Total Award Period Covered: 09/10/10 - 08/31/13 Location of Project: SUNY Potsdam Person-Months Per Year Committed to the Project. Cal:0.00 Acad: 0.00 Sumr: 0.00			
Support: <input type="checkbox"/> Current <input type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support Project/Proposal Title:			
Source of Support: Total Award Amount: \$ Total Award Period Covered: Location of Project: Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:			
Support: <input type="checkbox"/> Current <input type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support Project/Proposal Title:			
Source of Support: Total Award Amount: \$ Total Award Period Covered: Location of Project: Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:			
Support: <input type="checkbox"/> Current <input type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support Project/Proposal Title:			
Source of Support: Total Award Amount: \$ Total Award Period Covered: Location of Project: Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:			
Support: <input type="checkbox"/> Current <input type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support Project/Proposal Title:			
Source of Support: Total Award Amount: \$ Total Award Period Covered: Location of Project: Person-Months Per Year Committed to the Project. Cal: Acad: Summ:			

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Current and Pending Support

(See GPG Section II.C.2.h for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.	
Investigator: Andrew Lang	Other agencies (including NSF) to which this proposal has been/will be submitted.
<p>Support: <input type="checkbox"/> Current <input checked="" type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support</p> <p>Project/Proposal Title: Collaborative Research: Development and Preliminary Assessment of a Molecular Model Kit and other Chemistry Tools for Second Life</p> <p>Source of Support: NSF 0942743</p> <p>Total Award Amount: \$ 52,411 Total Award Period Covered: 06/01/10 - 05/30/12</p> <p>Location of Project: ORU/Drexel/Texas A&M Collaborative Proposal</p> <p>Person-Months Per Year Committed to the Project. Cal:0.00 Acad: 0.00 Sumr: 2.00</p>	
<p>Support: <input type="checkbox"/> Current <input type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support</p> <p>Project/Proposal Title:</p> <p>Source of Support:</p> <p>Total Award Amount: \$ Total Award Period Covered:</p> <p>Location of Project:</p> <p>Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:</p>	
<p>Support: <input type="checkbox"/> Current <input type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support</p> <p>Project/Proposal Title:</p> <p>Source of Support:</p> <p>Total Award Amount: \$ Total Award Period Covered:</p> <p>Location of Project:</p> <p>Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:</p>	
<p>Support: <input type="checkbox"/> Current <input type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support</p> <p>Project/Proposal Title:</p> <p>Source of Support:</p> <p>Total Award Amount: \$ Total Award Period Covered:</p> <p>Location of Project:</p> <p>Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:</p>	
<p>Support: <input type="checkbox"/> Current <input type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support</p> <p>Project/Proposal Title:</p> <p>Source of Support:</p> <p>Total Award Amount: \$ Total Award Period Covered:</p> <p>Location of Project:</p> <p>Person-Months Per Year Committed to the Project. Cal: Acad: Summ:</p>	

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

FACILITIES, EQUIPMENT & OTHER RESOURCES

FACILITIES: Identify the facilities to be used at each performance site listed and, as appropriate, indicate their capacities, pertinent capabilities, relative proximity, and extent of availability to the project. Use "Other" to describe the facilities at any other performance sites listed and at sites for field studies. USE additional pages as necessary.

Laboratory:

Clinical:

Animal:

Computer:

Office: 1 office for 3 people

Other:

MAJOR EQUIPMENT: List the most important items available for this project and, as appropriate identifying the location and pertinent capabilities of each.

Two servers

OTHER RESOURCES: Provide any information describing the other resources available for the project. Identify support services such as consultant, secretarial, machine shop, and electronics shop, and the extent to which they will be available for the project. Include an explanation of any consortium/contractual arrangements with other organizations.

Supplied by campus - air conditioning, UPS, etc. See appendix for agreement.

FACILITIES, EQUIPMENT & OTHER RESOURCES

FACILITIES: Identify the facilities to be used at each performance site listed and, as appropriate, indicate their capacities, pertinent capabilities, relative proximity, and extent of availability to the project. Use "Other" to describe the facilities at any other performance sites listed and at sites for field studies. USE additional pages as necessary.

Laboratory: The laboratory is equipped with glassware and instruments required to carry out the proposed work. This includes a thermostated bath capable of maintaining a constant temperature between -25 to 80C.

Clinical:

Animal:

Computer: Two computers are available for student use in the lab.

Office: Standard office space with necessary equipment (fax, scanner, printer) is provided.

Other:

MAJOR EQUIPMENT: List the most important items available for this project and, as appropriate identifying the location and pertinent capabilities of each.

Commonly used instruments to characterize compounds are available in the chemistry department at Drexel: 2 Varian NMR instruments (300 and 500 Mz), IR, UV and MS.

OTHER RESOURCES: Provide any information describing the other resources available for the project. Identify support services such as consultant, secretarial, machine shop, and electronics shop, and the extent to which they will be available for the project. Include an explanation of any consortium/contractual arrangements with other organizations.

FACILITIES, EQUIPMENT & OTHER RESOURCES

FACILITIES: Identify the facilities to be used at each performance site listed and, as appropriate, indicate their capacities, pertinent capabilities, relative proximity, and extent of availability to the project. Use "Other" to describe the facilities at any other performance sites listed and at sites for field studies. USE additional pages as necessary.

Laboratory:

Clinical:

Animal:

Computer: ORU provided laptop and desktop computers. Both are windows machines running Vista and are about two years old.

Office: ORU office approximately 60 sq. ft.

Other:

MAJOR EQUIPMENT: List the most important items available for this project and, as appropriate identifying the location and pertinent capabilities of each.

OTHER RESOURCES: Provide any information describing the other resources available for the project. Identify support services such as consultant, secretarial, machine shop, and electronics shop, and the extent to which they will be available for the project. Include an explanation of any consortium/contractual arrangements with other organizations.

CHEMISTRY NSF GRANT SERVICE LEVEL AGREEMENT

Introduction

The purpose of this document is to outline the Service Level Agreement (SLA) between Computing & Technology Services (CTS) and the National Science Foundation Grant administered by Dr. Martin Walker of the Chemistry Department (Grant) regarding CTS co-location and support of Wiki servers for the Grant. CTS may be referred to as the “Provider”, the Grant as the “Customer” and their constituents who make use of Grant Wiki Services as “Users” throughout this document. The scope of this contract is for two Wiki servers (servers) each being one rack unit in height (1U). Nothing in this document may supersede established policies.

Provider's Responsibility

- CTS will work with Customer to choose appropriate hardware for purchase when necessary.
- CTS will provide rack space for the servers in the Data Center including power with battery backup, physical security, monitoring, and climate control.
- CTS will install hardware and load OS on the servers to prepare them for configuration of the application software.
- CTS will install OS security patches and other patches as approved by the vendor.
- CTS will facilitate data backup according to CTS data classification guidelines.
- Working with vendors, CTS will provide hardware repair and maintenance (servers must be covered by a vendor provided hardware maintenance contract).
- CTS support is limited to server installation and configuration only and will not provide training or assistance as to the use of the application software.

Customer's Responsibility

- Customer is responsible for purchase of all hardware and software items, maintenance contracts, and vendor charges.
- Customer is responsible for any and all support or assistance to Users regarding the use of service.
- Customer agrees not to make any changes or install any upgrades that will affect the network without prior approval from CTS.
- Customer is responsible for administration and use of the application software.
- Customer agrees to the policy of limited controlled access to the Data Center for a designated number of individuals with CTS escort.

Fees/Pricing

Customer is responsible to provide annual cost reimbursement of \$2,500 per 1U server per year for co-location with support as outlined above. The Grant will be invoiced annually on or about January 1st. If the Grant’s Internet network traffic load and/or data backup requirements necessitate the growth of our existing campus infrastructure, customer will be subject to additional pricing fees accordingly. Charges will be reviewed with the customer prior to implementation. If the customer is unwilling or unable to fund the increase(s), the Provider reserves the right to limit backup space and network utilization at their sole discretion.

CHEMISTRY NSF GRANT SERVICE LEVEL AGREEMENT

Termination

Provider: The Provider may terminate this agreement for non-payment of the annual reimbursement or by mutual agreement with the customer, providing at least three (3) months notice to the Customer. The Customer may terminate this agreement at any time, providing at least thirty (30) days notice to Provider. Partial years will not be refunded due to customer termination.

Agreement Life

This agreement is considered perpetually binding. Provider reserves the right to increase the annual reimbursement based on increases in costs, CTS staff resources, or other factors.

Indemnification

Co-location service is provided by CTS “as is” with no warranties or guarantees expressed or implied. At no time is CTS liable for damage or losses incurred through use or misuse. The system will be periodically unavailable during periods of maintenance or outages. Maintenance schedules will be communicated ahead of time. The support provided by CTS will be during business hours only. This support will on a “Best Effort” basis (without any contractual response or resolution metrics). However, CTS maintains an enterprise-grade Data Center, which, in conjunction with active monitoring and notification systems, allows for sub-minute response time to problems during normal business hours.

SUNY Potsdam CTS Authorization:

Ali Shahidi, Director of Computing & Technology Services

Date

National Science Foundation Grant Administrator Authorization:

Dr. Martin Walker, Professor of Chemistry

Date



UNC
ESHELMAN
SCHOOL OF PHARMACY

THE UNIVERSITY
of NORTH CAROLINA
at CHAPEL HILL

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ALEXANDER TROPSHA, PHD
*K. H. Lee Distinguished Professor and Chair,
Director of the Laboratory for Molecular Modeling*

August 13, 2009

Prof. Martin A. Walker
Department of Chemistry
SUNY College at Potsdam
Potsdam, NY 13676 USA

Dear Martin:

I am very excited about your proposal under the NSF's STCI Program to create a wiki-based hub/nexus for chemistry. As a computational medicinal chemist I work at the interface between chemistry and biology (and between chemists and biologists!). This is a very challenging position because generally speaking both groups lack necessary complimentary knowledge due to their respective training. Ultimately, both groups would like to have a drug (most often, an organic molecule) emerging from their efforts, and in this regard an access to diverse chemical information that would become available in your proposed portal would be a critical resource. The unique aspect of your proposed portal is its interactive nature with respect to its users enabling the entire community of chemists to share their knowledge and learn from the experience of others.

I will be very happy to join the panel of your advisors should you proposal be funded. I wish you good luck with this important endeavor!

Sincerely,

Alex Tropsha

Alexander Tropsha, Ph.D.
K.H. Lee Distinguished Professor and Chair
MCNP Division
Director, the Laboratory for Molecular Modeling
Eshelman School of Pharmacy
UNC-Chapel Hill