S2015 CH-01 #16

Technology Fee RFP Worksheet

Use this form as a cover sheet for Full Proposals

(revised March 2014)

Semester &Year: **Fall 2014**	Date: **23 October 2014**	**$25,000.00**
Submitted by **Mark Eberhart**	Email Address: **Meberhar@mines.edu**	Ext: **3726**
Title of Proposal: **Computational chemistry and visualization software**		
Department/Organization: **Chemistry and Geochemistry**		

Budget Information

	Tech Fee Request	Direct Match* (Cash)	Total $ To Be Expended	Other Contributions (In kind, disc, etc)	Total Project Value
Equipment			0.00		0.00
Software	25,000.00	4,350.00	29,350.00		29,350.00
Maintenance			0.00		0.00
Operating & Supplies			0.00		0.00
Student Help			0.00		0.00
Other (attach detail)			0.00		0.00
Total……..	$25,000.00	$4,350.00	$29,350.00	$0.00	$29,350.00

*__Notes__: Direct. Match must be actual funds that are or will become available to be applied to direct expenditures. General department/organization technology operating or support costs are not appropriate. Work-study funds cannot be identified as matching funds. Use the "Other Contributions" column if applicable for faculty/staff/student time, vendor discounting beyond normal academic discounts, previous investments or purchases, and other in-kind contributions. *Documentation of matching fee expenditures must be provided to Technology Fee Account Manager as expenditures are made if a proposal is funded.*

The same matching funds cannot be used in more than one proposal (ie. If all proposals from a dept/organization are funded then the sum of all matching funds must be committed.)

Proposal Executive Summary

The National Science and Technology Council has proposed developing an educational framework that will promote a culture of integrated computational engineering. The Department of Chemistry and Geochemistry (CGC) recognizes an opportunity to build such a culture beginning with the introductory chemistry sequence required of all CSM students. While CGC has been exploring this possibility for almost a decade, the developments that now make this possible are fully quantum mechanical DFT codes that may be run on student computers and laptops and are equipped with robust user interfaces. While developing the expertise necessary to introduce this software into the first year courses, CGC and various research groups have together contributed roughly $10K/year to maintain a site license to such software. However, finding the funds is a year-to-year effort. The uncertainty associated with the continued availability to this software, has acted as a disincentive to its broader use, which will require many hundreds of man-hours to develop labs and other curricula for the first year courses.

We are requesting $25K from Tech Fees toward the $30K cost of three year ADF site license. Over this three-year period, we will phase the use of the software into our undergraduate program and particularly the first year sequence. We anticipate that this phase-in will be completed by fall 2017. At the conclusion of this period the Dean of the College of Applied Science and Engineering (CASE) has agreed, if we are sucessful with the phase in portion of this porposal, to find alternaitve sources for continued support of the annual license fee, possiblities include the use of lab fees, direct CASE support, or fees derived from lab manuals.

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This section must be fully completed for your proposal to be considered
Is this request part of a continuing project for which you have received previous technology fee awards? ☐ Yes ☒ No If yes, how many awards and how much funding have you received for this project during the past 3 years?
What is the proposed project lifetime or life expectancy of resources to be acquired? **3 years**
Where will the resources acquired be located? **Site license for software to be installed on machines in computer class rooms** Does this change the use of the existing space? ☐ Yes ☒ No If Yes, how is the space used now?
What impact will acquiring these resources have on cooling, power, and other building infrastructure? If there is any impact, the requirements must be discussed with Capital Planning and Facilities Management **None**
Will this project require additional network wiring or ports, have other impacts on the campus network, or involve the provision of wireless networking services in any way? ☐ Yes ☒ No If yes, you must coordinate those activities with the CCIT networking staff All wireless projects are subject to the campus wireless network infrastructure policy at **http://inside.mines.edu/UserFiles/File/PoGo/Policies/CIT/CIT_Wireless_Network_Infrastructure.pdf** If yes, explain:
Who will manage the resources? **CCIT (Sara Schwarz) and CGC (Mark Eberhart)**
Will other resources be retired or replaced if you receive this award? ☒ Yes ☐ No If yes, what do you propose to do with the old resources? **The software package Spartan will no longer be needed and we do not anticipate its continued use by Chemistry.**
Explain the impact on both departmental and central support staff as a result of acquiring these resources. Include in your discussion the consequences of reusing the old resources as well as the impact of acquiring new resources: **Assuming a new licensing structure is developed by SCM (see narrative) there will be minimal impact to the department. We have been coordinating up to 100 licenses on personal computers for three years and will continue to take responsibility for this task.**
What will the ***primary*** use of the requested resources be? **Education**
How many students per semester will use the requested resources? **up to 1200**
How many hours per week will the requested resources be committed to scheduled, supervised lab or classroom use? **During the rollout period, this will vary from 3 to 12 hours per week.**
How many hours per week will the requested resources be available in an open use / open lab environment? **168 hours/week**
Who will be permitted to use the resources (which students, in what classes or options, under what restrictions, etc)? **By year three of rollout, all CSM students will have access via personal computer. Please see narative for more information.**

The National Science and Technology Council (NSTC), the Cabinet-level council that coordinates science and technology across the Federal government recently identified policies intended to accelerate the pace of technological advance. These policies address, among other components, the need for a formal educational framework for both the undergraduate and graduate students who will pursue careers in industry and academia. This framework is needed by virtually all STEM related disciplines, where increasingly scientists and engineers are called upon to work in teams to develop and improve materials and implement these in engineering applications. In practical terms, students who will go on to make and engineer with materials must have enough training to understand materials modeling and theory, while modelers and theorists must understand the vocabulary and challenges confronting those who design with these materials. Fundamentally, the educational framework called for by the NSTC will promote a culture of integrated computational engineering.

The Department of Chemistry and Geochemistry (CGC) recognizes an opportunity to build such a culture beginning with the introductory chemistry sequence required of all CSM students. Just ten years ago, it would have been extremely difficult to offer a large number of undergraduate students access to chemical modeling tools and methods. However, advances in computational platforms, theory, and software, now make this objective both possible and desirable, making it possible to present chemistry as the modern integrated topic it is, where modeling and theory are used to illuminate and expand our understanding of the basic chemical principles underpinning all engineering fields.

While CGC has been exploring this possibility for almost a decade, the developments that now make this possible are fully quantum mechanical DFT codes with robust user interfaces and post processors that facilitate visualization and data analysis. Additionally, some of these software packages may be run on desktop and laptop computers. Even so, these codes are not toys and should not be thought of as an educational fad. These codes are serious pieces of laboratory equipment that will allow students to run computational experiments, and gain an appreciation for the ways that theory and modeling are being integrated into science and engineering at even the most basic level.

As mentioned, CGC has conducted scaled, trial programs, particularly in physical chemistry II (CHGN353), to develop curricula and the expertise and experience necessary to integrate theory and modeling into the first year offerings. In this process, we have evaluated several computational chemistry software packages including: Spartan, Gaussian, ADF and numerous types of freeware. Of these, ADF is the most appropriate, due in large measure to its efficiency—making laptops and other personal computers suitable computational platforms. The ability to perform serious modeling, in real time, on a readily available personal computer has proven to be the single most important factor to the success of our trial programs. Additionally, ADF has a user-friendly interface, and provides a larger and more robust set of post processor tools.

For the past several years CGC and various research group have together contributed roughly $10K/year to maintain an ADF site license. It is this license that has allowed us to run our trial programs. Though each year there is an element of uncertainty as to source of funds for the next year's site license.

While $10K is an exceptional expense to benefit the fifty or so students involved in pilots each year, it is a manageable and justifiable expense when spread across the 1200-1300

student who would be impacted by the widespread use of the software. Under such circumstances, it would be appropriate to use funds derived from other sources to cover the cost of the site license.

We are requesting $25K from Tech Fees toward the $30K cost of three year ADF site license. Over this three-year period, as outlined below, we will phase the use of ADF software into our undergraduate program and particularly the first year sequence. We anticipate that this phase-in will be completed by fall 2017, at which point the Dean of the College of Applied Science and Engineering (CASE) has agreed to find alternaitve sources for continued support of this resource, possiblities include the use of lab fees, direct CASE support, or fees derived from lab manuals. .

This software will impact seven chemistry courses with a combined yearly enrolment of over 2000 students. The greatest contribution to this enrollment comes from the first year sequence, consisting of three courses CHGN121, 122 and 125*. The software will also be used in the organic and physical chemistry sequence, with a combined yearly enrollment of more than 600 students.

Our plan calls for the introduction of the software in two modes. First, is its use in laboratory exercises (designated as Lab in the table below), requiring its installation in up to four computer classrooms. The second mode calls for the use of the software during class and for homework (designated as Lab/Lecture) and necessitating that the software be installed on student computers. We have experience with both modes of operation. The ADF software is available in CTLM B56 and for the past three years it has been installed on the personal computers of students taking CHGN353. Currently, the licenses are node locked, however, and this will pose difficulties as we expand to a larger number of classroom and personal computers. However, Scientific Computing and Modeling (the producers of ADF) have offered to work with us developing a floating license. We anticipate having the less cumbersome licensing structure in place by spring 2016.

	2015		2016		2017	
	Spring	Fall	Spring	Fall	Spring	Fall
CHGN121		Lab *100 students*		Lab/Lecture *250 students*		Lab/Lecture *800 students*
CHGN122			Lab *100 students*		Lab/Lecture *250 students*	
CHGN125	Lab *100 students*	Lab *100 students*	Lab/Lecture *250 students*	Lab *100 students*	Lab/Lecture *250 students*	Lab *100 students*
O-Chem CHGN223		Lab *200 students*		Lab *200 students*		Lab *200 students*
O-Chem CHGN224			Lab *200 students*		Lab *200 students*	
P-Chem CHGN351	Lab *50 students*	Lab *150 students*	Lab *50 students*	Lab *150 students*	Lab *50 students*	Lab *150 students*
P-Chem CHGN353	Lab/Lecture *50 students*		Lab/Lecture *50 students*		Lab/Lecture *50 students*	

The rollout plan for the ADF software. Dark blue grids indicate the course is not offered during that semester. The light blue grids indicate a trailing section

** Class currently operating as CHGN198*

Scientific Computing & Modelling

Scientific Computing & Modelling
TC • FEW • Vrije Universiteit
De Boelelaan 1083
1081 HV Amsterdam
The Netherlands

Colorado School of Mines
Accounts Payable
1500 Illinois Street
Golden, CO 80401
USA

PRO FORMA INVOICE

Invoice No: PF2014.09.15.2 **Invoice Date: 15 September 2014**
(Please contact sales@scm.com for final invoice)

Description	Amount	
Academic site license, 1 January 2015 - 31 December 2017		
ADF for unlimited cores	22,500.00	
BAND for unlimited cores	11,250.00	
ADF-GUI for 5 or more machines	8,100.00	
BAND-GUI for 5 or more machines	4,050.00	
DFTB for unlimited cores	12,600.00	
Total	58,500.00	
Combination discount (unlimited ADF + GUI)	-5,400.00	
Exchange rate discount	-5,310.00	
Multi-year discount	-3,186.00	
Total price excluding 3rd party	44,604.00	
Special Discount	-15,254.00	
MOPAC2012	0.00	
Total Amount Due	29,350.00	USD

Your reference:	E-mail dated 15 Sept. 2014
Our reference:	PF2014.09.15.2 A*B*Ga*Gb*D*M* 3yr
Your VAT number:	
Our VAT number:	NL 8072 70 143 B01
Payment terms:	30 days
E-mail for enquiries:	sales@scm.com

Payment by either of the following methods, in order of preference:

- By wire transfer to Bank of America, Chicago, IL, USA.
  Account number: 291006392013, Scientific Computing & Modelling NV
  For domestic (within the USA) transfers, the ABA routing number: 0260-0959-3
  The ACH routing number: 081904808
  For international payments, the SWIFT code: BOFAUS3N
- By wire transfer to ABN-AMRO, Amsterdam, Netherlands
  Account number: 536505632, Scientific Computing & Modelling NV
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  Netherlands

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