UNIVERSITY OF LOUISIANA AT LAFAYETTE

STEP Committee

Technology Fee Application

The Implementation of a Computational Chemistry Laboratory into Undergraduate Chemistry

Title

Dr. Barbara Marchetti

Name of Submitter
(Faculty or Staff Only)

Department of Chemistry

Organization

Title: Instructor Date: 08/02/2019
Name (Contact Person): Barbara Marchetti
Address: University of Louisiana at Lafayette, P.O. Box 43700, Lafayette, LA 70504
Phone Number: 337 482 5678 Email: barbara.marchetti1@louisiana.edu
Department/College/Org Chemistry

ABSTRACT (250 words or less):

The primary aim of this proposal is to secure funding for the design of a series of novel spectroscopy experiments for the undergraduate chemistry laboratories. Spectroscopy is a fundamental tool for chemical analysis which is routinely used in all fields of chemical, physical, medicinal and life sciences and finds application in both research and industrial purposes. Currently, our undergraduate chemistry laboratories are not equipped with the appropriate instruments which would allow our students to acquire fundamental practical skills in modern techniques and procedures routinely used in both an academic and industrial setting. As such, we propose to assemble a compact experimental set-up to perform spectroscopic analysis and photochemical experiments for various undergraduate chemistry laboratories such as the General Chemistry (CHEM115) and Physical Chemistry Laboratories (CHEM311). In addition, the use of the experimental set-up could be extended to undergraduate research CHEM362 and CHEM462 courses - providing students with a robust, modern and user-friendly analytical tool. The project requires a compact modular spectrometer (Avantes, AvaSpec-ULS2048XL-EVO) equipped with two pulsed broadband light sources (photoexcitation source and analysis source) and temperature-controlled cuvette holder for temperature dependent kinetics. The overall cost of the equipment is ~$14000. The set-up will allow for the acquisition of standard UV-Vis/NIR spectra, monitor fast reaction kinetics (~2 microseconds time resolution) at various temperatures and perform pump-probe experiments analogous to a flash photolysis (~6 microseconds time resolution).

3a. Purpose of grant and impact to student body as a whole

This grant application requests funds to purchase adequate equipment to construct various spectroscopy and photochemistry experiments for implementation into undergraduate chemistry teaching and undergraduate research laboratories. The basic experimental set-up includes a fiber-coupled, compact (and portable) modular spectrometer able to acquire spectra in the wavelength region 200 – 1100 nm. The spectrometer is coupled with a pulsed broadband deuterium-halogen light source (emitting 200-1100 nm). The light source is coupled to a fiber optic which delivers the light to the sample which located in a temperature-controlled cuvette holder. Such a cuvette holder acts as a thermostat which assures that the sample is at a constant temperature (in the range -30º C and 105º C): this feature is fundamental for acquiring temperature dependent kinetics of chemical reactions. The ultimate time resolution for the kinetics could be as short as 2 microseconds (minimum integration time allowed by the spectrometer). The assembly is arranged in a linear geometry, as in any standard UV-Vis-NIR spectrometer and allows to record transmittance/absorbance measurements. A second light source (Xenon lamp) is placed at a 90º orientation for photoexcitation of the sample and subsequent acquisition of emission spectra. In addition, synchronous use of both light sources can be used for broadband pump-probe experiments in which the excitation light source promotes a chemical reaction. In this case, the analysis light source allows for the acquisition of spectra changes and the reaction times associated with the photo-induced reaction. The set-up is controlled through a software package which allows complete computer-controlled operation. The whole system, including computational resources, is extremely easy to operate and user-friendly, which makes it suitable for teaching applications. These features allow for a broad flexibility of the assembly which makes it applicable to many laboratories – from general chemistry to more specialized courses (such as physical chemistry).

Similar experimental set-ups are routinely used in teaching laboratories in many universities, as they can be used in many applications, from basic science to chemical analysis for analytical and pharmaceutical purposes. The latter involves the identification and quantification of chemical substances and reaction products in mixtures (e.g. food analysis, pharmaceutical formulations and environmental samples), and the characterization of newly engineered materials. Due to the multi-disciplinary nature of such experiments, it is vital to provide our students with an adequate exposure to the range of cutting-edge methods which they will use in their future employment if chemistry remains their chosen vocation. In addition, the set-up includes a photoexcitation light source to investigate photo-induced chemical reactions. This option is not currently available in our laboratories but is a fundamental field of chemistry. Many possible photochemistry experiments can be implemented into undergraduate chemistry laboratories, such as kinetics of photoisomerization/photoreactions in photochromic compounds, flash photolysis to study radical reactions or photo-induced chemistry of inorganic catalysts. Providing students with training in an array of modern spectroscopic and photochemical methods will ensure that they can successfully graduate with the most complete portfolio of chemical skills that make them heavily competitive in the current academic and industrial market.

In order to implement the new spectroscopy and photochemistry experiments, we request funds for the purchase of one modular spectrometer (Avantes, AvaSpec-ULS2048XL-EVO) with a set of interchangeable slits, two broadband light sources (AvaLight-DHc and AvaLight-XE-HP), with fiber optic cables included and a temperature-controlled cuvette holder. The system is extremely versatile and can therefore be applied to a variety of laboratory courses while giving the students the opportunity of working with state-of-the-art equipment which is currently not available to them. The software is

provided with the equipment. Basic training is required for the fundamental operation of the set-up.

The new experimental assembly can be easily implemented into existing laboratory courses: CHEM115 (General Chemistry Laboratory), CHEM233 (Organic Chemistry Laboratory), CHEM252 (Inorganic Chemistry Laboratory) and CHEM311 (Physical Chemistry Laboratory). In addition, the set-up could be made available to students registered for undergraduate research courses (CHEM362 and CHEM462) if necessary.

To conclude, we strongly believe that the implementation of new, state-of-the-art equipment for undergraduate chemistry laboratory into our current program is paramount to ensure that our students are exposed to the highest level of modern tools and skills available in chemistry.

3b. Projected lifetime of enhancement

The instrument is robust and reliable. The typical lifetime of a spectrometer is ~10-15 years. Minor replacement components could involve new light bulbs for the light source or new fiber-optic cables (if damaged).

3c. Person(s) responsible for:

i. Implementation: Dr. Barbara Marchetti is an expert in spectroscopy and photochemistry. She will be responsible for the implementation of the new equipment in her laboratory courses. She is available to train other instructors for the use of the instruments in other chemistry laboratory courses.

ii. Installation: The set-up is very compact and portable, as such it does not require any particular handling precautions. In addition, no particular storage conditions are required.. No expert external installation is necessary. An installation and maintenance manual are also provided with the equipment for further support.

iii. Maintenance: The maintenance of the set-up may include (i) periodic updates to the operation software, (ii) change of lamp bulbs in the light sources and (iii) replacement of fiber optic cables. Dr. Barbara Marchetti will be in charge of maintaining the set-up in an operating state. No expert external maintenance is required. A maintenance manual is provided when purchasing the equipment.

iv. Operation: Dr. Barbara Marchetti will also develop a series of instructions to aid in the operation of the spectrometer by other educators and students. In addition, Dr. Barbara Marchetti will construct and advise on a series of experiments which can be carried out on the spectrometer and applied to all fields of chemistry, such as organic, analytical and physical chemistry. The set-up will be available to any educator at the Department of Chemistry who is in need for a fast and precise spectrometer for a teaching laboratory experiment. Instructors will have access to the installation, maintenance and operation manuals if any further assistance is necessary.

v. Training: Dr. Barbara Marchetti is an expert in the use of spectroscopic experiments and has operated similar and more complex equipment in her previous appointments. She will ensure that every

instructor has access to the spectrometer and light sources and that they are well prepared to train students to use it. Dr. Marchetti will compile a set of instructions for students to follow, in order to sufficiently operate the equipment. As with normal laboratory sessions, instructors will provide additional support for students.

Budget Proposal

1.	**Equipment**	**$**	**13,792.10**
2.	**Software**	**$**	**0**
3.	**Supplies**	**$**	**0**
4.	**Maintenance**	**$**	**0**
5.	**Personnel**	**$**	**0**
6.	**Other**	**$**	**0**
TOTAL:		**$ 13,792.10**	

d. Budget narrative

Equipment:
One Avantes SensLine spectrometer (AvaSpec-ULS2048XL-EVO), one compact full-range deuterium-halogen light source (AvaLight-DHc) with power supply and one full-range, high power, pulsed Xenon lamp (AvaLight-XE-HP) with power supply, one temperature-controlled cuvette holder, one quartz fluorimetric cuvette.

Software:
AvaSoft spectroscopy software (provided free of charge with the equipment)

Supplies:
No supplies required

Maintenance:
No maintenance funds required

Personnel:
No personnel funds required

Other:
None

The quotation from the company (Avantes) is reported below (item 9 should not be included in the total requested amount)

Company Address	500 S Arthur Avenue Suite 500 Louisville, CO 80027 US	Created Date	7/15/2019
		Expiration Date	8/30/2019
		Quote Number	19564
Phone	303-410-8668		
Email	infousa@avantes.com		
Prepared By	Ryan Flaherty	Contact Name	Barbara Marchetti
Phone	(303) 410-8668	Phone	barbara.marchetti1@louisiana.edu
Email	r.flaherty@avantes.com	Email	
Fax	(303) 410-8669		
		Ship To Name	University of Louisiana at Lafayette
Bill To Name	University of Louisiana at Lafayette		
Bill To	Lafayette, LA 70503		

Line Item	Product	Description	Quantity	Sales Price	Discount	Total Price
1	AvaSpec-ULS2048XL-EVO-RS-UA	Ultra Low Straylight Fiber Optic VIS/NIR with Replaceable Slit spectrometer,2048 pixel 14x500µm Backthinned CCD detector, grating UA (200-1160nm), DCL-UV/VIS-200, OSC-UA, USB powered, high speed USB3 and ETH interface. including Avasoft-Full and SLIT-KIT-SMA (slit-25-RS preinstalled; 50, 100, 200um in box).	1	$5,320.00	5.00%	$5,054.00
2	AvaLight-DHc	Compact deuterium-halogen light source, 200-2500 nm with TTL shutter, needs extra PS-12V/1.25A	1	$1,998.00	5.00%	$1,898.10
3	PS-12V/2.08A	Power Supply for Avalight-HAL-(S)-Mini	2	$70.00	5.00%	$133.00
4	IC-DB26-2	Interface cable AvaSpec-USB2 platform to DB15 for AvaLight-S with shutter for auto save dark/ lamp off, AvaLight-XE control	2	$100.00	5.00%	$190.00

5	CUV-UV/VIS-TC-ABS/FL	Temperature controlled cuvette holder fluorescence & absorbance kit, two QILUV imaging lens assemblies, two QCL-UV collimating lens ssemblies,..two QMP mirror plugs, BATH 100 submersible pump, QSLITS optical slits, cover with access cap, tubing, cables...	1	$4,800.00	5.00%	$4,560.00
6	Avalight-XE-HP	Xenon light source (200-1000 nm), needs interface cable and extra PS-12V/1.0A power supply	1	$1,270.00	5.00%	$1,206.50
7	CUV-10-4	Quartz cuvette, 10 mm, 4 windows, 3.8 mm	1	$310.00	5.00%	$294.50
8	FC-UVIR400-1-BX	Fiber cable, 400 µm fiber, broadband UV/VIS/NIR (250-2500nm) ,1 m., SMA Terminations; BX stainless steel jacketing	3	$160.00	5.00%	$456.00
9	FH-INL-1"	Inline filterholder for 1" filters, max 60mm optical path, incl 2 collimating lenses and SMA connectors	1	$860.00	5.00%	$817.00

Thank you for the opportunity to serve your instrumentation needs!
Quotes are in USD and valid for 30 days
Standard delivery is UPS Ground, FOB Origin

Subtotal	$15,378.00
Total Price	$14,609.10
Grand Total	$14,609.10

Full terms and conditions are available upon request by contacting Avantes at the number above.