UNIVERSITY OF MISSISSIPPI

Notice of Intent to Certify Sole Source

SS 014

The University of Mississippi (UM) anticipates purchasing the item(s) listed below as a sole source purchase. Anyone objecting to this purchase as a sole source shall follow the procedures outlined below.

Commodity or commodities to be purchased (manufacturer, model, description):

Horiba Scientific – LabRAM HR Evolution Raman Microscope

The need to be fulfilled by this item(s) and why it is the only one that can meet the specific needs of the department:

This is the only instrument that can be used for this research. This is the instrument named in our National Science Foundation (NSF) award # CHE-1532079, and the award requires this specific instrument.

We currently have a Horiba HG-2S Raman spectrometer, which is an older version of the requested instrument and compatibility is important.

High resolution is critical to our experiments. We study spectral shifts on the order of 1 cm-1 and require this for our work. See, for example,

A. A. Howard, G. S. Tschumper, and N. I. Hammer, "Effects of Hydrogen Bonding on Vibrational Normal Modes of Pyrimidine," Journal of Physical Chemistry A, 114, 6803-6810 (2010). DOI: 10.1021/jp101267w

B. A. M. Wright, L. V. Joe, A. A. Howard, G. S. Tschumper, and N. I. Hammer, "Spectroscopic and Computational Insight into Weak Noncovalent Interactions in Crystalline Pyrimidine," Chemical Physics Letters, 501, 319-323 (2011). DOI:10.1016/j.cplett.2010.11.046

C. K. L. Munroe, D. H. Magers, and N. I. Hammer, "Raman Spectroscopic Signatures of Noncovalent Interactions Between Trimethylamine N-oxide (TMAO) and Water," Journal of Physical Chemistry B, 115, 7699-7707 (2011). DOI: 10.1021/jp203840w

D. A. M. Wright, A. A. Howard, J. C. Howard, G. S. Tschumper, and N. I. Hammer, "Charge Transfer and Blue Shifting of Vibrational Frequencies in a Hydrogen Bond Acceptor," Journal of Physical Chemistry A, 117, 5435-5446 (2013). (cover article) DOI: 10.1021/jp401642b

Getting close to the laser line (within 10cm-1) for the study of low every modes in newly developed nanomaterials is also critical to the use of this instrument.

In addition, this instrument is the only one that has been found that has the required following capabilities:

1. For flexibility, stability and throughput, it is required that the Raman system consist of one main unit integrating all components, microscope, spectrograph, lasers and detectors into a single hard coupled unit for maximum rigidity and stability. The use of light guides or fiber coupling is not acceptable.

2. Spectral resolution is a very important performance consideration in a Raman/PL microscope as it determines how precisely close together spectral peaks can be resolved and how small a frequency shift can be measured when monitoring stress/strain of material and pressure and temperature induced shifts. The system should therefore have a spectral resolution dispersion of 0.2cm-1/pixel at 532nm and 0.75cm-1/pixel at 244nm when using a 2400g/mm grating and 26 micron pixels CCD.

3. We require the instrument to be capable to operate over a wide wavelength range, from UV-VIS-IR. Some of this range is required now and some with range extensions via future upgrades. The instrument must, therefore, be capable to operate between 200-1500nm and be fully achromatic (without chromatic shift). Reflective optics are required to avoid any achromatism issues and allow to cover the full range with optimum focusing on intermediate optics including the confocal hole and detector, to insure best spatial and spectral resolution at all wavelength. This operation must be obtained without requiring a change of spectrograph optics. Any required detectors for this range must be capable of being simultaneously mounted on the instrument. Any kind of manual exchange of detectors or spectrometer optics is not acceptable.

4. The system should have the capability to access to Raman frequencies using 633nm HeNe laser down to 5 cm^{-1} in principle (at least 10 cm^{-1} with the specific components) with a single stage monochromator as this preserves high throughput advantage ideally suited for mapping and low scattering samples. The system should also allow measuring the entire Raman/PL range from 400 to 2500 nm.

5. The system must be supplied with a spectrograph with a minimum pathlength of 785mm or higher capable of accommodating 3 detectors simultaneously, in order to cover the full range from UV to IR (200nm to 2200nm), using a CCD detector for 200-

1000nm, with an option for an InGaAs detector for best efficiency in the range 950nm-1500nm, and a further option for extended InGaAs to cover up to 2200nm.

6. For ease of operation and maximum sample measurement throughput the system must be fully automated via software. All hardware selections must be accessible and operated via software this includes but is not limited to:

a. All lasers – minimum of 4 selectable by software – but no limit to the number of lasers allowable.

b. All filters – minimum of 4 selectable by software but no limit to the number of filters allowable.

c. All detectors up to 3 selectable by software

d. Neutral density filters up to 9 positions

e. Video camera operation - laser, white light and Raman selection

f. Raman scanning and central wavelength position

g. Spectrometer slit

h. Fully variable, automated confocal pinhole

i. Raman mapping, xy.

j. Switching between microscope measurement and remote measurement via a fiber probe if option is included

7. Exact positioning and measurement of very small particles and features is important for Raman measurements. The system must therefore be provided with a video camera and focusing optics for the video camera to allow observation of both the laser spot on the sample and the sample under white light illumination simultaneously for exact positioning of features at the laser spot for Raman measurement.

8. In order to adequately control the laser power at the sample the system should have a neutral density filter wheel with a minimum of 9 position (100%, 50%, 25%, 10%, 5%, 3%, 1%, 0.1%, 0.01%) controlled by software, working from 400 nm to NIR.

9. A multichannel air cooled (-70°C) CCD detector with the minimum of 1024 x 256 pixel front illuminated chip 1” wide, including MPP readout for optimum noise performance. The CCD must cover the Spectral range: 400-1100 nm. TE cooling to -70C or better is required for reduced dark noise. The system should be able to acquire data from the whole 1 inch of the CCD chip, in both stationary and extended scanning modes, without producing spectral artifacts or aberrations in the data such as vignetting. The

system must also be capable of accommodating liquid nitrogen cooled detectors if required for future upgrades.

10. Scanning: The instrument provided must allow spectra to be acquired in stationary AND a continuous scanning mode. Step and stitch methodologies alone are not sufficient as these introduce artifacts. The continuous scanning facility must allow Raman spectra to be scanned across and read from the CCD in multiples of pixels AND sub-divisions of pixels (to enhance spectral band-shape).

11. Confocal Raman measurements: Confocal measurements are a key feature of any Raman microscope. The system must provide optimum confocality using an actual true confocal aperture and allow for the confocal measurement volume to be set using a continuously variable automated pinhole. At 488nm the system must provide a lateral confocal resolution of better than 0.5 micron and an axial confocal resolution of better than 1.5 microns. The use of combined slit and CCD aperturing is not acceptable as this does not allow for the spectral resolution to be independently set from the confocal resolution. The confocal volume should be continuously variable through software control and allow the confocal volume (e.g. pin-hole size) to be varied while the Raman signal readout is being automatically cycled. This is required to allow the Raman signal from a small area to be optimized in real time. The system must allow programmed automated confocal Raman measurements to be taken with stepped (different) confocal hole sizes. This must be achieved without requiring operator intervention between each measurement.

12. The system will be used to measure Raman spectra of weak scattering materials, in addition the feature sizes and consequent sampling volume in these materials can be very small so the Raman signal will consequently be very weak. To optimize instrument throughput and measurement sensitivity (spectral S/N) the system must use the laser/Raman filter in injection/rejection mode. Therefore for maximum sensitivity the filters must operate in injection/rejection mode i.e. the same filter reflects the laser in to the microscope AND rejects the Rayleigh and laser scattered light that is reflected back in to the spectrometer. These filters MUST be guaranteed for a minimum of five years. Use of a separate beamsplitter and the filter in only transmission mode is not acceptable as this dramatically reduces the instrument throughput by up to four times.

13. The cut-off of any visible and 785nm Raman filters must be better than $50cm^{-1}$ (all measured at 50% transmission).

14. Hyperspectral Imaging: The instrument must have the capability to provide hyperspectral images at a high spectral resolution. Therefore the system should be available with XY mapping capabilities. An automated mapping stage should provide a step-resolution of at least 0.1 microns. The instrument software must drive the mapping stage and allow the acquisition of hyperspectral images. Exact positioning of

the sample and mapping area is required – therefore an image capture card and video camera should be used to visualize the sample and be coupled through the system software. The software must also allow the visualization and mathematical manipulation of hyper-spectral images. It must be possible to generate images of band intensity, position and width.

15. Fast Mapping: The instrument will be used to generate large area hyperspectral maps/images. Therefore in order to minimize the time required for these maps, when the Raman signal from our samples allow, the system must provide fast mapping for the rapid generation of Raman maps/images. The system should allow a per pixel spectral measurement time as short as 5ms/pixel. This means that a Raman map/image with 10,000 pixels would take 50 seconds. The software must allow for real time generation and display of the Raman images using either band fitting or modeling during the acquisition

16. The system must have a polarization module that allows the user to rotate the polarization of the laser and to analyze the polarization of the Raman signal. For both modules, the angle have to be adjustable with at least 1 degree precision and computer controlled.

17. The system should have the capability to measure samples using standard 10mm x 10mm cell or NMR tubes for easy macro, liquid and headspace measurements. It should be pre focused and require no tools or adjustment and ideally attaches directly to the microscope turret. A mirror should be used for multi pass measurements to increase sensitivity.

18. A temperature controlled stage should be included: Fully computer controlled and integrated into the main Raman system control software for ease of use with a temperature range: -196C to 600C. Suitable long working objectives should also be provided to allow for the window thickness of the temperature cell.

Name of company/individual selling the item and why that source is the only possible source that can provide the required item(s):

Horiba Scientific is the only vendor for this instrument as it is custom-built and sold directly.

Submission Instructions and Format of Response from Objecting Parties:

Interested parties who have reason to believe that the item(s) above should not be certified as a sole source should provide information in the following format for UM to use in determining whether or not to proceed with awarding the Sole Source purchase.

1.1 **Interested Party Information**

1.1.1 **Contact Name, Phone Number, Address and email address**

1.1.2 **Company Website URL, if applicable**

1.2 **Objection to Sole Source Certification**

1.2.1 **Interested parties must present specific objections to the Sole Source certification using the criteria listed above.**

1.2.2 **A statement regarding the Interested Party's capabilities as related to this Sole Source Certification Request.**

1.3 **Comments will be accepted at any time prior to Tuesday, October 20, 2015 at 3:00 pm (Central Time) to Katherine Jones at kajones4@olemiss.edu (with Cc: to purchase@olemiss.edu) at The University of Mississippi Procurement Services Department, 164 Jeanette Phillips Drive, PO Box 1848, University, Mississippi 38677. Responses may be delivered by hand, via regular mail, overnight delivery, or e-mail. The envelope or email should reference the sole source number. UM WILL NOT BE RESPONSIBLE FOR DELAYS IN THE DELIVERY OF RESPONSES. It is solely the responsibility of the Interested Parties that responses reach UM on time. Interested Parties may contact Katherine Jones to verify the receipt of their Responses. Responses received after the deadline will be rejected.**

If after a review of the submitted notice and documents, UM determines that the commodity in the proposed sole source request can be provided by another person or entity, then UM will withdraw the sole source certification and submit the procurement of the commodity to an advertised competitive bid or selection process.

If UM determines after review that there is only one (1) source for the required commodity, then UM will appeal to the Public Procurement Review Board for approval to purchase.