Department Chemistry, University of Kerala, Kariavattom, Thiruvananthapuram, Kerala, India – 695 581

14/08/2020

<u>E-Tender Notice (Re-tender)</u>

Department of Chemistry, University of Kerala, Kariavattom invites open tenders through e-Procurement (in two bid system), from reputed manufacturers/authorized distributors/Indian Agents for the purchase of the equipment 'Material Software' in the Department, in connection with the implementation of the Specific Project "Advanced Research Laboratory for Molecular Sensing and imaging".

Last date and time for submission of tender online	21/08/2020: 5 PM	
Date and time of opening of Technical	26/08/2020: 11AM	
bid		
Date and time of opening of Financial	After technical Evaluation.	
bid		
For technical details contact	Dr. Sony George	
	Assistant Professor and Head Department of Chemistry	
	Mobile : +91-9446462933	
	Email : emailtosony@gmail.com	

TECHNICAL SPECIFICATIONS

A software that is required to provide a complete modelling and simulation environment which enable the researcher to predict and understand the relationships of atomic / molecular structure of a material with its properties and behavior. The software must consist of:

1. Validated and efficient quantum mechanical applications based on Density Functional Theory (DFT), hybrid QM/MM and semi-empirical methods. Quantum mechanical methods yield accurate thermodynamic, kinetic and structural results, providing an efficient input to experiment and insight into processes at the atomic level. Accurately prediction of molecular and crystal geometry, chemical reaction pathways, optical properties, spectra (IR, Raman, NMR, EELS, ELNES, XES, XANES, EXAFS etc). The quantum mechanical tools should consists of different modules with following simulation capabilities:

• Offers simulation capabilities such as accurate prediction of phonon spectra, dielectric constants, and optical properties. Simulate the properties of solids, interfaces, and surfaces for a wide range of materials classes, including ceramics, semiconductors, and metals, with this premier density functional theory (DFT) quantum mechanical code and an improved implementation of the Density Functional based Tight Binding (DFTB) quantum simulation method for the study of electronic properties of materials containing hundreds of atoms.

• Combine computational speed with the accuracy of quantum mechanical methods to predict materials properties reliably and quickly.

• Access Gaussian's broad range of *ab initio* modeling methods via the easy-to-use graphical interface.

• Predict NMR chemical shift tensors, isotropic shifts, and electric field gradients for any material

• Accurately treat systems such as grain boundaries, nanoclusters and protein-ligand complexes with the quantum mechanics-based program designed specifically for calculations on large systems of more than 500 atoms.

• Combine the accuracy of quantum mechanics with the speed of a force field calculation to perform calculations on very large systems in a cost and time effective manner.

• Predict fundamental properties, such as sorption isotherms and Henry's constants needed for investigating separations phenomena. It must also be able to find the most stable adsorption sites for a broad range of materials.

• Rapid calculation of physical and chemical properties of molecular organic and inorganic systems.

- 2. A graphical user environment-in which user can construct, manipulate and view models of molecules, crystalline materials, surfaces, polymers, and mesoscale structures. This is to be complemented by a complete set of solution methods including quantum, atomistic, classical, mesoscale, and statistical that enable user to evaluate materials at various particle sizes and time scales. The software should allow user **to easily build, modify, visualize and simulate a wide range of materials including** molecular and inorganic crystals with following simulation capabilities:
 - Easily build and visualize many different materials types from organometallic complexes to polymers, crystals, surfaces, and catalysts.
 - Identify compounds with optimal physicochemical properties for Quantitative Structure-Activity Relationships and extend the base tools to include a neural networks model building method and accurate quantum mechanical descriptors.

*Internationally well known brands such as material studio, Q-Chem etc. are preferred.

Terms and Conditions

- 1. Every tenderer should submit Tender fee of Rs. 2,500/-.
- 2. Every tenderer should submit Earnest Money Deposit (EMD) of Rs.18,000/-.
- 3. The bidder shall have executed "Similar Nature" of single order for an amount not less than Rs.50 lakhs in last three financial years in Government Department/PSU/Autonomous Body or any reputed organization. References order copy along with proof of completion certificate for the project must be provided.
- 4. Quantities can be increased or decreased by purchaser and bidder has to supply deviated quantities at the rates prescribed and approved by the purchaser in the tender document. Purchase of optional items will be finalized at the time of financial evaluation. However, the bidder must quote the optional items. The bidder should quote all items, partial quote will not be accepted.
- **5.** Original Equipment Manufacturer (OEM) Certificate/ Undertaking. If the bidder is not an OEM, Certificate of authorized dealership/ distributorship from the OEM. A Certificate from the OEM for technical support to the bidder and supply of spares.
- **6.** Incomplete & conditional tenders and tenders received after the due date will be summarily rejected without assigning any reasons thereof.
- 7. Commercial bids of Short–listed vendors will only be opened. Please note that the Vendor(s) who do not qualify in the technical bid will not be considered for commercial bid.
- 8. The bidder must not sub-contract the work to other providers.
- **9.** The prices quoted must be on "all-inclusive till destination" basis. The prices quoted should be inclusive of all Taxes Freight, Packing & Forwarding Charges, Handling, Delivery Charges, installation charges etc.
- **10.** The configuration given is the minimum configuration that is/are required. Vendors may choose to supply higher/better/ enhanced systems/peripherals, but their financial quotes shall be treated as if they have been offered for the specified configuration only.
- **11.** The Bidder shall bear all the costs associated with the preparation of the documents, submission of its bid and we will in no case be responsible or liable for these costs, regardless of the conduct or outcome of the bidding process.
- **12.** The bid shall be typed and shall be signed by the bidder or a person duly authorized to bind the bidder to the contract.
- 13. The bid shall contain no interlineations erasures or overwriting except as necessary to correct

errors made by the Bidder. In such case the person or persons signing the bid shall initial such corrections.

- 14. The bidder is expected to examine all instructions, forms, terms, condition, and technical specifications in the tender Documents. Failure to furnish all information required by the tender Documents or submission of a bid not substantially responsive may result in the rejection of its bid.
- **15.** The bidders shall give undertaking that all the Components used in the equipment's shall be original make as per the technical specifications submitted and the hardware/software shall be supplied with the authorized license certificates, if found contrary the supplier shall replace the component/equipment with original one at their own cost.
- **16.** Validity of tender: Tender submitted shall remain valid at least for 90 days from the date of opening the tender. Validity beyond three months from the date of opening of the tender shall be by mutual consent.
- 17. Delivery and installation: Proposed delivery schedule should be mentioned clearly. Delivery and installation should be made at Department of Chemistry, University of Kerala, Kariavattom Campus Trivandrum 695581, without any extra cost. Complete installation, testing and demonstration of the system and day to-day maintenance are to be provided at site. The Supply and installation of items must be made within four weeks from the date of issue of supply order. Delay in supply will lead to penalty @1% of the value of tender for every week of delay or part thereof. (i.e. exceeding three days will be calculated as one week). If it is found that the items so supplied are not as per supply order specifications, the supply made will be rejected and Earnest Money Deposit will be forfeited.
- 18. Warranty period will start from the date of successful installation of all the items at site.
- **19.** Service facility: Supplier should mention their details of service setup and manpower in Trivandrum who are responsible for after sales support.
- **20.** In case of any dispute, the decision of the University authority shall be final and binding on the bidders. The undersigned reserves the right to reject any or all of the tenders received without assigning any reason thereof.

Documents to be uploaded:

- 1. Signed Compliance Matrix
- 2. Detailed Technical Brochure
- 3. BoQ
- 4. Detailed Financial Bid in pdf format

Registrar