

**Indian Institute of Technology
Department of Chemical Engineering**

Nov 5th, 2013

Purchase of *ab-initio* Quantum Mechanical Modeling Software

Quotations are invited for minimum **two user license (which can run up to a total of 20 calculations at a time) of *ab-initio* quantum mechanical modeling software** with minimum specifications given in the Table below. Technical and commercial bids must be submitted in **separate** sealed envelopes subscribed with “Technical Bid” or Commercial Bid” as appropriate. Both technical and commercial bids should be enclosed in an envelope subscribed “Quotation for Material Studio software”.

The quotation should reach **Dr. M. Ali Haider, Department of Chemical Engineering, IIT Delhi, Hauz Khas, New Delhi – 110016**. Mention NIQ Ref No and Item description (title) on top of your quotation.

Last Date of submission: 22/11/2013

S. No.	Item	Description
1	Modules	<ol style="list-style-type: none">1. The software should include modules (codes) that can carry out density functional theory (DFT) calculations using (a) plane wave basis set, (b) numerical orbitals (c) semi-empirical quantum mechanical method2. Modules should have latest quantum mechanical tools that can implement DFTB (tight binding) and linear scaling DFT3. It should have ability to implement a combined QM/MM approach.
2	Visualizer	<ol style="list-style-type: none">1. Visualizer has ability to create and manipulate crystals, polymer, nanotubes and molecular structures.2. It can generate and analyze charge densities, density of states, vibrational frequencies.3. The crystal manipulator is able to generate structure with vacancies and doping that can be used directly in DFT codes.4. The visualizer has integrated capacity to generate structures to be used as input for transition state calculations.
3	Additional features	<ol style="list-style-type: none">1. Codes for carrying out classical simulations like molecular dynamics and mechanics to predict conformations, VLE diagrams, mixture compatibility, sorption of gases in frameworks.2. An integrated platform for carrying out mesoscale simulations.3. Analyse diffraction patterns from X-Ray, electron and neutron and solve crystal structure, as well as predict crystal morphologies.4. Tools for carrying out Quantitative Structure Activity

		Relationships using descriptors generated by above tools.
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Terms and Conditions:

1. The delivery period should be clearly indicated in the quotation.
2. Submitted quotations should clearly mention the validity period, preferably for a minimum of 3 months.
3. Guaranty or warranty period should be specified.
4. The mode of payment should be clearly indicated.
5. All other general terms of delivery should be specified with quotation.
6. The quotation should include details of the pricing for each items along with the Special discounts, packing, forwarding. Inland Freight and Export documentation charges.
7. The item should be properly packed with clear mention of name of manufacturer/name of supplier along with date.
8. Payment will be done under EFT (Electronic Fund Transfer) / RTGS (Real Time Gross Settlement) scheme after receipt of item. It is compulsory required that the seller should be registered for RTGS at IIT Delhi.
9. IIT Delhi is exempted from paying custom duty under notification No.51/96 (partially or fully) and necessary "Custom Duty Exemption Certificate" can be issued after providing following information.
 - a. Shipping details i.e. Master Airway Bill No. and House Airway No. (if exists)
 - b. Forwarder details i.e. Name, Contact No., etc.

Custom Duty Exemption Certificate will be issued to the shipment in the name of the Institute and Bills of Entry should be submitted to IIT Delhi later on.
10. Either the Indian agent on behalf of the Principal/OEM or Principal/OEM itself can bid but both cannot bid simultaneously for the same item/product in the same tender. If an agent submits bid on behalf of the Principal/OEM, the same agent shall not submit a bid on behalf of another Principal/OEM in the same tender for the same item/product.
11. If the bidder is an authorized dealer of any manufacturer, the authorized Indian dealership certificate from the principles should be enclosed. Similarly, proprietary certificate for proprietary items should be provided.
12. IIT Delhi is exempted from paying Excise Duty and necessary Excise Duty Exemption Certificate will be provided for which following information are required.
 - a. Quotation with details of Basic Price, Rate & Amount on which ED is applicable.
13. Please quote the price of the imported item at FOB (Freight on Board) IIT Delhi inclusive of all taxes, freight, delivery, installation and onsite training charges. The quotation should provide the total price of the system including all taxes and transportation charges.

14. In case IIT Delhi is imposed with demurrage charge due to import on CIF, the entire demurrage charge has to be borne by the Indian Agent of foreign supplier.
15. Three years comprehensive warranty be provided and AMC price beyond 3 years should be mentioned separately.
16. Delivery period: within 1 month from the issue of supply order.
17. The quotations must have validity of at least three months.
18. The products will be used for educational purposes. Any applicable academic institution discounts should be offered and stated clearly.
19. Authority of IIT Delhi reserves the right to reject any or all quotations without assigning any reasons.

Dr. M. Ali Haider,

Department of Chemical Engineering,

IIT Delhi