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Inquiry No. **IITK/CHM/TGG/2016/002**

Last date: 4<sup>th</sup> May, 2016 till 1:00 PM

Extended last date: 10<sup>th</sup> May, 2016 till 1:00 PM

Sub.: Request for quotation for **“Simulation software for electronic and transport properties of inorganic and organic material on surface and interface”**

Dear Sir/Madam

Kindly send us sealed quotation for the following item. Quotation should be addressed to **Dr. Thiruvancheril G. Gopakumar, Department of Chemistry, IIT Kanpur 208016**, and must reach on or before 10<sup>th</sup> May, 2016 till 1:00 PM.

Thanking you

Thiruvancheril G. Gopakumar

**Specifications for Simulation software for electronic and transport properties of inorganic and organic material on surface and interface**

**Methods:** DFT, Semi-Empirical, and Classical, Classical potentials, Abinit

**Computation:** Electronic structure, Electron transport, Phonon transport, Thermal properties, Thermo-electric properties, Optical properties, Mechanical properties, Transistor characteristics

**Analysis Tools:** 3D visualizations, isosurfaces, Band structure and DOS, projected DOS, trajectory analysis, Generate movie, Plots with math operations, Save output in all image formats.

**Miscellaneous:** a) Tool for generation molecules, surface, interfaces, crystals and transport electrodes

b) Write possibility of own plug-in

c) Graphical user interface for other software packages like VASP

d) Export atomic structures to all common file formats

**Terms and Conditions:**

1. Delivery: Via electronic delivery (Download from corresponding website)
2. Nature of service: Electronic