

INDIAN INSTITUTE OF TECHNOLOGY KANPUR
Department of MSE

Enquiry no.: MSE/AKS/ICMNH/LTA/2020/001

Enquiry Date: 14/02/2020

Closing date: 23/02/2020

Sealed quotations should reach the undersigned latest by 12 noon on 23rd February, 2020.

Description	Quantity
VASP Software (for academic institutions upto 6 users)	1

The above-mentioned software should conform to the following specifications:

1. The Software should calculate the electronic structure and chemical and physical properties of materials at the atomic scale using Density Functional Theoretical Calculations that is from the First Principles Simulations based Projector-Augmented Plane-wave based technique.
2. The potentials must be supplied as library based the so-called PAW method
3. The Software should also be capable of handling time-averaged molecular dynamics simulation based on Born-Oppenheimer approximation (BOMD) also lattice dynamics.
4. The Software should be both OpenMP and MPI compatible for High-Performance computations and simulations and should be the fore-front as the leading code in Materials Discovery HPC Simulations.
5. The Software should be compatible for varieties of compilers.

Terms and conditions:

1. The supplier should provide the source code.
2. The supplier should provide the technical support as and when needed as appropriate.
3. The supplier should supply the updates at least up to the first three years for the program when available.
4. Quotations should have a validity of a minimum of 60 days.
5. Technical specification along with the extent of compliance should be mentioned.
6. Quotations that do not provide the extent of compliance with our requirement will be rejected.
7. Permissible educational discount should be provided since the software will be used for research work of students.
8. IIT Kanpur is exempted from payment of Excise Duty under notification no. 10/97

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