



भारतीय प्रौद्योगिकी संस्थान (भारतीय खनि विद्यापीठ), धनबाद

धनबाद, झारखण्ड, भारत, पिन-826004

(शिक्षा मंत्रालय, भारत सरकार के अधीन राष्ट्रीय महत्व का एक संस्थान)

INDIAN INSTITUTE OF TECHNOLOGY (INDIAN SCHOOL OF MINES), DHANBAD

DHANBAD, JHARKHAND, INDIA, PIN-826004

(An Institute of National Importance under Ministry of Education, Govt. of India)

PROJECT PURCHASE SECTION Phone: (0326)2235660 || Email: projectpurchase@iitism.ac.in || Website: www.iitism.ac.in

No. CY-PRJ-030-26-27

Date: 7 August 2026

Request for Quotation

To,

Subject: Permanent License for the use of VASP software, releases 5 and 6.6, by academic institutions for 6 users free updates for 3 years.

Sir,

Indian Institute of technology (Indian School of Mines), Dhanbad is interested in the purchase of the materials/equipment/service listed below:

Sl. No.	Detailed Specifications	Quantity
1	Permanent License for the use of VASP software, releases 5 and 6.6, by academic institutions for 6 users free updates for 3 years. (Specification in Annexure –II)	01 No

INSTRUCTIONS:

- 1) Please attach relevant technical literature of the item.
- 2) Please attach authorization certificate for OEM.
- 3) Price Basis: FOR IIT (ISM) Dhanbad
- 4) The items/ materials shall be required to be delivered at Department of Chemistry and Chemical Biology of IIT (ISM) Dhanbad at the risk and cost of the tenderer.
- 5) ***Please attach a certificate that the quoted price is not more than that of any other Govt. organization/ institution in India. This has to be mentioned in the offer letter clearly.***
- 6) The rates should be quoted for each item separately as per price schedule attached as annexure I
- 7) The items/ materials shall be required to be delivered at Chemistry and Chemical Biology Department of IIT (ISM) Dhanbad at the risk and cost of the tenderer.
- 8) Your tender must be **valid for minimum 180 days** from the date of opening of tender.
- 9) Full details of items/materials offered should be given in the tender along with supporting & relevant literatures/ Technical Literature.
- 10) Tender may please be submitted ***in sealed cover only superscribed with Enquiry No. CY-PRJ-030-26-27 latest by 05.09.2026.***
- 11) acceptance/Installation. The performance security will be refunded without any interest, provided that the performance is satisfactory.
- 12) The offer must be submitted in the office of Deputy Registrar (Purchase & Stores), IIT (ISM), Dhanbad–826004 (Jharkhand, India) only. Please send your offer by Registered Post/ Speed Post/ Courier along with Courier receipt. Tender/ quotation will be received during IIT (ISM) Dhanbad working hours only (i.e. Monday to Friday). At any circumstances by hand delivery is not acceptable. Late or delayed tenders shall be summarily rejected. Bids sent through Email/Fax or submitted in unsealed cover(s) will not be accepted and such bids will be treated as non-responsive bids.
- 13) Any other information that you may like to obtain, you are free to contact IIT (ISM) Dhanbad before submission of tender.
- 14) IIT (ISM) Dhanbad reserves the right to accept and/or to reject any/all tenders without assigning any reason.
- 15) **Payment:** Payment shall normally be made within 3-4 weeks subject to satisfactory supply, submission of tax invoice and delivery challan in triplicate (as per Purchase Order Terms) of the ordered materials/items. ***Advance payment is not admissible.***
- 16) You are requested to fill the enclosed **Annexures**.



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- 17) **Please attach purchase order copies of the same equipment which you have supplied to any other Govt., public sector and autonomous institutions.**
- 18) **a) In a tender, either the Indian agent on behalf of the principle/ OEM and the Principle/OEM itself can bid but both cannot bid simultaneously for the same item/product in the same tender.**
b) If an agent submit bid on behalf of the principle/ OEM, the same agent shall not submit a bid on behalf of another principle/ OEM in the same tender for the same item/product.

**For and on behalf of
IIT(ISM), Dhanbad**

Deputy Registrar
(Project Purchase Section)
O/o Dean (R&D)



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Annexure –I(A)

1. PRICE SCHEDULE FOR GOODS BEING OFFERED WITHIN INDIA

Name of the Bidder _____

NIT Reference No. _____

File Reference No. _____

Sl. No.	Full Description of items with (HSN Code/SAC Code)	Quantity	Unit Price (in INR)	Total Amount (in INR)
1.				
2.				
3.				
Ex-Works Price-				
Packing & Forwarding				
Transportation				
FOR (IIT ISM) Dhanbad				
GST/IGST (their rate(s) as the case may be, clearly specified)				
<u>Please note that IIT ISM is eligible for Concessional GST as per Notification No. 45/2017-Central Tax (Rate) for CGST, 45/2017-State Tax (Rate) for SGST and 47/2017-Central Tax (Rate) for IGST.</u>				
Insurance up to Destination/handover (in case of fabrication)				
Installation & Commissioning charge				
Training charges, if any				
Additional Warranty Charges, if any				
Annual Maintenance Charge, if any				

*(On the basis of the technical specifications submitted)

Total Bid Price _____

in words _____

Note :

(a) The Price schedule of optional items shall be indicated in a separate sheet in the same Performa.

(b) Cost spare parts may be indicated separately

Signature of Bidder

Name _____

Business

Address _____



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Annexure- 1(B)

2. PRICE SCHEDULE FOR GOODS BEING OFFERED FROM ABROAD

Name of the Bidder _____

NIT Reference No. _____

File Reference No. _____

Sl. No.	Description/Part No./Make Model	Quantity	Unit Price (in foreign currency)	Total Amount (in foreign currency)
1.				
2.				
3.				
Total Ex-Works Price-				
Packing & Forwarding and inland freight				
*FCA (at port)				
Terminal charges, loading on vassal				
**FOB (name of port)				
Air freight & insurance up to destination port				
*CIF				
Carrier charges & insurance up to final destination				
**CIP				
Concessional Custom Duty (Against DSIR Certificate)				
IGST rate (Against IIT (ISM) Certificate)				
Other Duties taxes/clearance charge, if any				
Transportation charges up to IIT ISM Dhanbad				
Chargeable weight/Gross weight of consignment				
Indian agency Commission (%)				
Installation & Commissioning charge				
Training charges, if any				
Additional Warranty Charges, if any				
Annual Maintenance Charge, if any				
Educational discounts, if any				

* & ** Mandatory requirement

Total Bid Price in words _____

Note :

Total Bid price in foreign currency _____ in words

(a) Indian agent name & address _____

(b) Installation, commissioning & training charges, if any _____

(c) Please note that Indian agents' commission shall be paid in Indian Rupees only.

(d) Banker's details such as- Name of account holder, Account Number, Name of Bank, Branch code, RTGS code, NEFT code, SWIFT code etc.

(f) Price schedule of optional items shall be indicated in a separate sheet in the same performa.

(g) Quoting Price for FOB/FCA and for CIF/CIP basis, otherwise bid will be rejected.

(h) Wherever the price quoted on FOB/FCA and CIF/CIP basis are the same, the contract would be made on CIF/CIP basis only.

(i) Country of Origin Dimension and Gross Weight must be provided.

Signature of Bidder

Name _____

Business Address _____



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Annexure –I(C)

SELF-CERTIFIED DECLARATIONS FOR TAKING PART IN TENDER

a. Regarding blacklisting / debarring

b. Insolvency

1. I / We _____ (Tenderer) hereby declare that the firm / agency / Company, namely M/s _____ has not been declared as **insolvent**.

AND

2. I / We _____ (Tenderer) hereby declare that the firm / agency / Company, namely M/s _____ has not been **blacklisted or debarred** in the past by Union / State Government or Organization from taking part in Government tenders in India.

OR

2. I / We _____ (Tenderer) hereby declare that the Firm/Agency/Company, namely M/s _____ was **blacklisted or debarred** by Union/ State Government or any Organization from taking part in Government tenders for a period of _____ years w.e.f. _____ to _____. The period is expired and now the Firm/Agency/Company is entitled to take part in Government tenders.

In case the above information is found to be false I / We are fully aware that the tender/contract will be rejected / cancelled by Director, IIT(ISM) Dhanbad, and EMD shall be forfeited.

In addition to the above the Director, IIT(ISM) Dhanbad will not be responsible to pay the bills for any completed/partially completed work.

Date:

Place:

Self Certification: _____

Name: _____

Address: _____

Stamp:



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Annexure –I(D)

UNDERTAKING

(To be signed and submitted/uploaded along with technical bid documents on Company's Letter Head)

(As per Office Memorandum No. F.7/10/2021-PPD (1) dated: 23.02.2023 issued by Department of Expenditure (Ministry of Finance), Govt. of India)

Model certificate for Tenders

"I have read the clause regarding restrictions on procurement from a bidder of a country which shares a land border with India; I certify that this bidder is not from such a country or, if from such a country, has been registered with the Competent Authority. I hereby certify that this bidder fulfills all requirements in this regard and is eligible to be considered. [Where applicable, evidence of valid registration by the Competent Authority shall be attached]"

Place:

Signature: _____

Date:

Name: _____

Stamp: _____

OR

Model certificate for tenders for work involving possibility of sub-contracting

"I have read the clause regarding restrictions on procurement from a bidder of a country which shares a land border with India and on sub-contracting to contracting from such countries I certify that this bidder is not from such a country or, if from such a country, has been registered with the Competent Authority and will not sub contract any work to a contract form such countries unless such contractor is registered with the Competent Authority. I hereby certify that this bidder fulfills all requirements in this regard and is eligible to be considered. [Provide Compliance for the above in Vendor Specified Commercial Terms.]"

Place:

Signature: _____

Date:

Name: _____

Stamp: _____



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Annexure-II

Technical Specifications for Procurement of Vienna Ab initio Simulation Package (VASP)

1. Name of the Software

Vienna Ab initio Simulation Package (VASP)

2. Type of Software

Scientific Computational Software for **First-Principles Density Functional Theory (DFT)** Calculations.

3. Purpose

The software will be used for first-principles electronic structure calculations based on **Density Functional Theory (DFT)** and beyond-DFT methods to investigate the structural, electronic, magnetic, optical, thermodynamic, and catalytic properties of materials. The software will support research in Energy storage materials, Lithium-ion, Sodium-ion, Magnesium-ion, Calcium-ion, and Aluminum-ion batteries, Hydrogen evolution reaction (HER), Oxygen evolution reaction (OER), CO₂ reduction, Semiconductor materials, Nanomaterials, Catalysis, Metal-organic frameworks (MOFs), MXenes, Two-dimensional materials, Surface science, Defect engineering, Photocatalysis, Spintronics, Computational chemistry, and Computational materials science.

4. Technical Specifications

The software should satisfy the following minimum specifications.

4.1 General Requirements

Latest stable release of Vienna Ab initio Simulation Package (VASP), commercial academic license, Linux compatible, source code should be provided, MPI parallel execution support, OpenMP parallelization support, hybrid MPI/OpenMP execution capability, installation on HPC clusters, support for Intel and AMD processors, support for InfiniBand communication, and support for modern compilers including Intel OneAPI and GNU Compiler Collection (GCC).

4.2 Electronic Structure Methods

The software should implement Density Functional Theory (DFT), spin-polarized DFT, non-spin-polarized DFT, Generalized Gradient Approximation (GGA), Local Density Approximation (LDA), Meta-GGA, hybrid density functionals, Hartree–Fock exchange, DFT+U, van der Waals corrected functionals, Spin–Orbit Coupling (SOC), and non-collinear magnetism.

Supported exchange-correlation functionals should include, but not be limited to, PBE, RPBE, PBEsol, SCAN, revSCAN, HSE03, HSE06, B3LYP, where applicable, LDA, and PW91.

4.3 Pseudopotentials

The software should support the Projector Augmented Wave (PAW) method, complete PAW potential library, standard, soft, and hard PAW datasets, scalar relativistic potentials, and spin–orbit compatible potentials.

4.4 Structural Optimization

The software shall perform geometry optimization, atomic relaxation, cell optimization, volume optimization, variable cell relaxation, equation of state calculations, and elastic constant calculations.

4.5 Molecular Dynamics

Support should include Ab initio Molecular Dynamics (AIMD), NVE ensemble, NVT ensemble, NPT ensemble, Langevin dynamics, Nose–Hoover thermostat, Parrinello–Rahman dynamics, and temperature-controlled simulations.



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4.6 Electronic Properties

The software should calculate band structure, Density of States (DOS), partial DOS, charge density, difference charge density, electron localization function (ELF), Bader charge compatible outputs, work function, electrostatic potential, and local density of states.

4.7 Optical Properties

Capability for dielectric function, optical absorption spectra, reflectivity, refractive index, and Electron Energy Loss Spectra (EELS), Optical conductivity.

4.8 Magnetic Properties

Support for ferromagnetic systems, antiferromagnetic systems, ferrimagnetic systems, magnetic moments, spin density, non-collinear magnetism, and spin-orbit coupling.

4.9 Vibrational Properties

The software should perform phonon calculations, vibrational frequency calculations, force constant calculations, thermodynamic property calculations, finite displacement calculations, and provide interface compatibility with Phonopy.

4.10 Surface and Interface Calculations

Support for surface slab models, adsorption energy calculations, surface reconstruction, vacancy defects, grain boundaries, heterostructures, and interface modeling.

4.11 Transition State Calculations

The software should support Nudged Elastic Band (NEB), Climbing Image NEB (CI-NEB), transition state search, and diffusion barrier calculations.

4.12 Advanced Methods

Support for GW approximation, Bethe-Salpeter Equation (BSE), time-dependent calculations, where available, Random Phase Approximation (RPA), Berry phase calculations, polarization calculations, piezoelectric properties, and ferroelectric calculations.

4.13 High Performance Computing

The software shall support large-scale parallel computations, distributed memory architecture, shared memory architecture, hybrid MPI/OpenMP execution, efficient scalability on HPC clusters, multi-node parallel execution, and high processor count calculations.

4.14 File Compatibility

The software should support POSCAR, CONTCAR, OUTCAR, INCAR, KPOINTS, CHGCAR, WAVECAR, XDATCAR, EIGENVAL, PROCAR, DOSCAR, LOCPOT, and vasprun.xml.

4.15 Visualization Compatibility

The software outputs should be compatible with VESTA, OVITO, VASPKIT, pymatgen, ASE (Atomic Simulation Environment), Phonopy, Bader Charge Analysis, VTST tools, and Python scripting interface.

5. Licensing Requirements

The license should include an Institutional Academic License, latest stable version, source code access, perpetual license for the purchased version, software updates as per vendor policy, installation support, documentation, user manual, and technical support.

6. Operating System

The software should support Linux 64-bit, CentOS, Rocky Linux, Ubuntu, and Red Hat Enterprise Linux.

7. Hardware Compatibility



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Compatible with Intel Xeon processors, AMD EPYC processors, HPC clusters, multi-core CPU architecture, high-speed InfiniBand networks, and large-memory compute nodes.

8. Applications

The software will be used for electronic structure calculations, material design, catalyst screening, surface chemistry, battery materials, hydrogen storage materials, carbon capture materials, semiconductor materials, metal oxides, two-dimensional materials, nanoclusters, MXenes, MOFs, zeolites, photocatalysts, magnetic materials, superconductors, defect engineering, computational catalysis, and renewable energy materials.

9. Deliverables

The vendor shall provide the licensed software package, source code, PAW potential datasets, installation guide, user manual, license certificate, installation assistance, technical support during installation, and access to software updates according to the license agreement.

10. Warranty and Support

The vendor shall provide installation support, technical assistance, bug fixes, software updates during the support period, email-based technical support, and online documentation.

11. Compliance

The software should be an officially licensed version supplied by an authorized distributor or directly by the developers. The software should comply with the licensing policies of the VASP developers and be suitable for installation on the institution's High-Performance Computing (HPC) cluster.

Justification

The **Vienna Ab initio Simulation Package (VASP)** is one of the world's leading first-principles simulation packages for computational materials science. It employs Density Functional Theory (DFT) with the Projector Augmented Wave (PAW) method and plane-wave basis sets to accurately predict the structural, electronic, magnetic, optical, and thermodynamic properties of materials. VASP is extensively used in high-impact research involving batteries, catalysis, nanomaterials, semiconductors, hydrogen storage, photocatalysis, and quantum materials. Procuring an institutional academic license will enable advanced computational research, support funded projects, and strengthen high-performance computing capabilities within the institute.