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PROPRIETARY ARTICLE NOTICE

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1. Indian Institute of Petroleum and Energy (IIPE), Visakhapatnam is an autonomous institute under the Ministry of Petroleum & Natural Gas, Govt. of India. The Institute would like to purchase **"VASP (Vienna Ab initio Simulation Package) Software"** on proprietary basis.

2. The following documents are uploaded to open information, to submit objections, comments if any from any manufacturer regarding proprietary nature of the equipment/item:-

   i) Proprietary Certificate by the firm.

   ii) Details of the Software package.

3. Objections if any are to be submitted through e-mail to procurement@iipe.ac.in within 7 days from the date of publishing this notice, failing which it will be presumed that no vendor is having any comments to offer and the case will be processed on merits.

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INDIAN INSTITUTE OF PETROLEUM & ENERGY ★ VISAKHAPATNAM ★

Proprietary Certificate

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Vienna 2023-02-13

Proprietorship Confirmation for VASP

Dear potential VASP customer,

It is hereby confirmed that the VASP Software GmbH has the unrestricted and perpetual right to license the Vienna ab initio simulation program (VASP), including the pseudopotential and PAW data base, the documentation, as well as any other data and programs distributed with the VASP software.

The VASP Software GmbH and Materials Design S.A.R.L. for Europe, the Middle East and Africa and Materials Design, Inc. for the North, Central and South Americas, Australia and Asia and their official local distributors are the sole distributors of the VASP software worldwide. A complete list of approved Distributors and Partners of Materials Design can be found at https://www.materialsdesign.com/distributors-and-partners.

With best regards,

Vasp Software GmbH

Prof. Dr. Georg Kresse
managing director of the VASP Software GmbH

INSTITUTE OF PETROLEUM & ENERGY
VISAKHAPATNAM

Details of the Software Package

Permanent License for the use of VASP software , release 5 and 6.3 by acadmic institutions for 6 users free updates for 3 years.

Vienna Ab intio Simulation Package (VASP) :-

The Vienna Ab initio Simulation Package (VASP) is a computer program for modeling materials at the atomic scale, e.g. computing electronic structure and quantum mechanical molecular dynamics, from first principle. VASP computes an approximate solution to the many-body Schrödinger equation, in Density Function Theory (DFT), by solving the Kohn-Sham equations or in the Hartree-Fock (HF) approximation, by solving the Roothaan's equation. Hybrid functions that combine the Hartree-Fock approach with density function theory are also implemented. In addition, Green's functional methods (quasiparticles GW and ACFDT-RPA) and multiple-body perturbation theory (Møller-Plesset of order 2) are available in VASP. Vienna Ab initio Simulation Package (VASP) is the leading electronic structure program for solids, surfaces and interfaces. VASP is an extremely well tested, powerful and proven program for computations based on Local and Semi-Local Density Function Theory (DFT) applying elementary plane wave sets. In addition, VASP provides advanced methods beyond DFT to calculate electronic structure and response, as well as energy with very high precision.

Software should give output to the following properties of the materials

- Total electronic energy of any 3D periodic arrangement of atoms
- Forces on atoms, pressure, and stress tensors
- Collinear and non-collinear magnetic moments
- Equilibrium lattice parameters and atomic positions as obtained from energy, force, and stress minimization
- Hyperfine splitting
- Electric field gradients and quadrupolar coupling constants
- NMR chemical shifts
- Solvation effects for surfaces and molecules
- External electrostatic field effects
- Ab-initio molecular dynamics: nVE, nVT, npT ensembles, simulated annealing, averages, uncertainties, and trajectories
- Energy band structure: accurate band gaps, dopant levels, and band offsets based on hybrid functionals, and GW methods
- Total and partial (atom and orbital momentum projected) electronic density of states
- Electronic charge and spin density, electrostatic potential, and Bader charge analysis

- Work functions
- Response functions including dielectric and piezoelectric tensors
- Born effective charges and Γ-point phonon modes
- Optical spectra: dielectric function and conductivity, reflectivity, refractive index, transmission, absorption, attenuation and extinction coefficients as well as emissivity as a function of frequency, total emissivity vs. temperature, color spaces for D65 and FL2 spectral distributions of illuminants (CIELAB)

Jobs to perform

- Plane-wave based electronic structure method for periodic structures
- All-electron method with projector augmented wave (PAW) potentials for all elements from H to Cm, including a set for highly accurate excited states
- Scalar- and fully-relativistic, spin-orbit coupling
- A variety of Van-der-Waals functionals, including BEEF-vdW and SCAN + rVV10
- DFT-D2/D3 (Grimme), DFT-dDsC, and Tkatchenko-Scheffler force-field based correction for van-der-Waals and dispersion forces and energies
- Density functional theory (DFT) with local (LDA) and gradient- corrected (GGA) semi-local functionals: AM05, PBEsol, PBE, rPBE, BLYP, etc.
- Hybrid functionals: HSE06, PBE0, B3LYP, and dielectric-dependent hybrid functionals with the mixing parameter for non-local exchange being determined from the dielectric function. In addition, screened exchange and Hartree-Fock.
- Meta-GGA functionals: revTPSS, TPSS, SCAN, MS2, MS1, MS0, M06-L, modified Becke-Johnson LDA
- Optical response functions from DFT, hybrid functionals or GW
- Electron-hole interactions (excitonic effects) from time-dependent hybrid functionals or solving the Bethe-Salpeter equation on top of GW4
- Accurate total energy, forces, and zone center phonon modes from adiabatic connection fluctuation dissipation theorem and the random phase approximation (ACFDT-RPA)5, automatic optimization of atom positions based on ACFDT-RPA
- Space-time algorithm for computing the polarizability for GW and ACFDT-RPA6, which scales mostly cubic rather than quartic with system size, thus enabling simulations for much larger systems
- Accurate total energy from Moeller-Plesset perturbation theory
- Density functional perturbation theory