



MGU INNOVATION FOUNDATION

(Section 8 Company under the Companies Act, 2013)

MAHATMA GANDHI UNIVERSITY

Priyadarsini Hills, Kottayam – 686560

Phone: 0481- 2992684, Website: www.mguif.org



Tender No: MGUIF/PUR/03/2023-24

Date: 06/10/2023

TENDER NOTICE

Sub: - The Chairman, MGU Innovation Foundation (MGUIF), Mahatma Gandhi University Campus, Kottayam, invites two cover online bid (Technical & Financial bid) from reputed firms for Phase- II development of MGU Innovation Foundation which includes ***Supply, installation, and setting up of Synopsys Quantum ATK with NEGF- Materials and Device Simulation Software with a RHEL Perpetual License at MGU Innovation Foundation, Mahatma Gandhi University Campus.*** The period of the tender is 30 days from the date of tender.

Tender documents and other tender details can be downloaded from the website: <https://etenders.kerala.gov.in>

SI No	Description of Tender	
1.	Tender No	MGUIF/PUR/03/2023-24
2.	Scope	Supply, installation, and setting up of Synopsys Quantum ATK with NEGF-Materials and Device Simulation Software with a RHEL Perpetual License at MGU Innovation Foundation, Mahatma Gandhi University Campus.
3.	Cost of Bid Document	Rs. 2,550/- (Rupees Two Thousand Five Hundred Fifty Only) + GST (Non-Transferable and non-Refundable)
4.	Earnest Money Deposit (EMD)	Rs.17,000/- (Rupees Seventy Thousand Only)
5.	Tender publishing date	06-10-2023
6.	Last Date of Receipt of the Tender	14-10-2023 up to 5:00 PM
7.	Date of Opening Technical Bid	16-10-2023 at 03:30 PM
8.	Mode of Submission of Bid	The Tender details and documents can be viewed & downloaded by login into https://etenders.kerala.gov.in .
9.	Address	The Chairman, MGU Innovation Foundation, Mahatma Gandhi University Campus, Kottayam, Kerala- 686560.
10.	Contact Details	Phone: 0481- 2992684 E mail: purchase@mguif.com
11.	Validity period	60 Days
12.	Period of supply and installation	60 Days

Note: General tender documents and tender schedule can be downloaded in A4 plain size paper free of cost from the website www.etenders.kerala.gov.in

**SYNOPSIS QUANTUM ATK WITH NEGF- MATERIALS AND DEVICE SIMULATION
SOFTWARE WITH A RHEL PERPETUAL LICENSE**

Technical Specification: -

Standard Academic Bundle for Nano simulation (5 Simulations)

(Floating License, All licenses on single cluster, Perpetual License)

- ✓ 5 Licenses of Quantum ATK (DFT/Semi-empirical) + NEGF
- ✓ 5 Licenses of ATK Master Forcefield (Classical)
- ✓ 2 Licenses of VNL (GUI)
- ✓ 2 Licenses of VNL Links (VASP Interface)
- ✓ 256 MPICH Slaves for faster simulation

Product Specific Features:

1. Quantum-mechanical computational methods.
1.1. LCAO-based Density Functional Theory (DFT).
1.1.1. Numerical atomic orbital basis sets (SIESTA type)
1.1.2. Inclusion of indirect atom pairs for improved accuracy
1.1.3. Norm-conserving Troullier-Martins pseudopotentials
1.1.4. FHI/HGH/OMX/SG15 potentials provided for almost all elements of the periodic table, including semicore potentials for many elements.
1.1.5. OMX and SG15 potentials are fully relativistic
1.1.6. DFT+1/2 method.
1.1.7. Ghost atoms (vacuum basis sets) for higher accuracy in the description of surface and vacancies.
1.1.8. Virtual crystal approximation (VCA)
1.2. Plane wave DFT method.
1.2.1. HSE06 exchange-correlation functional.
1.3. Semi-empirical tight binding
1.3.1. Extended Hückel Calculator.
1.3.2. Slater-Koster Calculator.
1.3.3. DFTB-type model.
1.3.4. 30 different parameter sets are shipped with the product, and more can be downloaded and used directly.
1.3.5. Built-in Slater-Koster models for group IV and III-V semiconductors.
1.3.6. Extended Hückel model with over 300 basis sets for (almost) every element in the periodic table.
1.3.7. Spin-orbit interaction (parameterized).
1.3.8. Flexible and customizable verbosity framework to control the level of output to the log files
2. Classical empirical potentials.
2.1. Force Field.
2.1.1. Over 280 bond-order potentials included.
2.1.2. Two/three-body potentials: Lennard-Jones (various versions), Coulomb (various versions), StillingerWeber, Tersoff (various versions), Brenner, Morse, Buckingham, Vessal, Tosi-Fumi, user-defined tabulated.
2.1.3. Many-body: EAM, MEAM, Finnis-Sinclair, Sutton-Chen, charge-optimized many-body (COMB).

2.1.4.Support for custom combinations of potentials.
2.1.5.Parallelized via OpenMP for optimal multicore performance (MPI parallelization in implementation).
3. Electrostatic models
3.1. Poisson equation solver
3.1.1.FFT (for periodic systems)
3.1.2.Two solvers for systems including metallic/dielectric regions:
3.1.2.1. Multigrid
3.1.2.2. Conjugent gradient method (parallelized in memory and execution)
3.1.3.FFT2D solver for transport systems.
3.1.4."Direct" solver for large-scale calculations (parallelized in memory)
3.1.5.Multipole expansion for molecules.
3.1.6.Metallic and dielectric screening regions.
3.1.6.1. Allows for computation of transistor characteristics (gated structures) as well as charge stability diagrams of single-electron transistors.
3.1.7.Local atomic shifts.
3.1.7.1. Simulate external fields.
3.1.8.Implicit solvent model.
3.1.9.Support for charged systems.
4. NEGF method for two-probe systems.
4.1. Non-equilibrium Green's function (NEGF) description of the electron distribution in the scattering region, with self-energy coupling to two semi-infinite leads (source/drain electrodes).
4.2. Open boundary conditions (Dirichlet/Dirichlet) allows application of finite bias between source and drain for calculation of I-V curve.
4.3. Includes all spill-in contributions for density and matrix elements.
4.4. Use of electronic free energy instead of total energy, as appropriate for open systems.
4.5. Ability to treat two-probe systems with different electrodes (enables studies of single interfaces like metalsemiconductor or p-n junctions, for instance).
4.6. Ability to add electrostatic gates for transistor characteristics (see above under "Electrostatic models").
5. Surface Green's function method for single surfaces.
5.1. NEGF description of the surface layers, with self-energy coupling to a semi-infinite substrate (replaces the slab approximation with a more physically correct description of surfaces).
5.2. Appropriate boundary conditions for infinite substrate and infinite vacuum above the surface, both for zero and finite applied bias on the surface.
6. Performance and stability options.
6.1. Scattering states method for fast contour integration in non-equilibrium (finite bias).
6.2. O(N) Green's function calculation and sparse matrix description of central region.
6.3. Double or single semi-circle contour integration for maximum stability at finite bias.
6.4. Ozaki contour integration to capture deep states.
6.5. Sparse self-energy methods to save memory.
6.6. Options to store self-energies to disk, either during calculation (instead of RAM) or permanently, to reuse in other calculations.
6.7. Adaptive (non-regular) k-point integration for transmission coefficients.
7. Calculation of I-V curves.
7.1. Elastic, coherent tunneling transport
7.2. Quasi-inelastic (LOE) and fully inelastic (XLOE) electron-phonon scattering.
7.2.1.Works with any combination of methods for the electronic and ionic degrees of freedom (DFT, tightbinding, DFTB, classical potentials).
7.2.2.Many performance options, such as averaging over phonon modes (bunching), using energy dependent relaxation energies, and repeating the density matrix for homogeneous systems.

7.2.3. Inelastic transmission spectrum (IETS) analysis.
7.3. Special thermal displacement (STD) approximation to efficiently capture the effect of phonon scattering on the I-V curve by creating a canonical average over all phonon modes.
8. Deep-level analysis of transport mechanisms
8.1. Transmission coefficients (k-point/energy resolved)
8.2. Monkhorst-Pack or edge-to-edge zone filling k-point scheme, or sample only part of the Brillouin zone for detailed information updated in 2016
8.3. Spectral current
8.4. Transmission spectrum, eigenvalues, and eigenchannels
8.5. Device density of states, also projected on atoms and angular momenta
8.6. Voltage drop.
8.7. Molecular projected self-consistent Hamiltonian (MPSH) eigenvalues
8.8. Current density and transmission pathways
8.9. Spin-torque transfer (STT) for collinear/non-collinear spin
8.10. Atomic-scale band diagram analysis via LDOS or device DOS
9. Transport properties of fully periodic systems.
9.1. Complex band structure.
9.2. Bulk transmission spectrum.
10. Machine-Learned (ML) Force Fields Moment Tensor Potentials (MTPs)
10.1. 100-1000x faster generation of realistic structures of complex multi-element crystalline, amorphous materials & interfaces, defect and dopant migration barriers, thermal transport, crystallization vs. DFT.
10.2. Systematically improvable MTPs
10.3. Active learning MTP simulations to automatically add DFT training data during molecular dynamics (MD) simulations.
10.4. Employ provided MTP potentials for Si or develop potentials for new materials and problems using automated training and simulation workflows
11. Complex Semiconductor Materials, Interfaces & Gate Stacks
11.1. Use ML MTPs for obtaining realistic crystalline, amorphous materials, interface, gate stack structures, simulating dopant diffusion, thermal transport, and crystallization
11.2. Plot band edges in projected DOS, local DOS and projected local density of states analysers.
11.3. Defect and dopant simulation improvements.
12. 1D & 2D-Material Based FETs.
12.1. More accurate band diagrams and device I-V characteristics with the new HSE06-NEGF methodology compared to PBE-NEGF.
12.2. More accurate on-state calculations using Neumann boundary conditions in the transport direction compared to Dirichlet at the Semi-Empirical level.
12.3. Up to 80% faster simulations of gated devices with vacuum regions using the new Poisson solver using a non-uniform grid compared to the parallel conjugate gradient (PCG) solver.
13. Advanced Surface Process Simulations.
13.1. Enhanced surface process simulation module enabling scanning over a range of impact energies and incident angles of “shooting” atoms at a surface for maximum yield in sputtering, etching (ALE) and deposition (ALD) processes.
13.2. Use the newly implemented thermochemical selectivity analysis tools in the GUI to screen critical reactions in a process, find ideal reactants and optimal reaction conditions for the processes.
13.3. Compute quantities, such as sputtering yield and sticking coefficient, needed for feature scale and reactor scale models.

TERMS AND CONDITIONS: -

1. The product should have Lifelong warranty.
2. Installation, Training/Familiarization and commissioning of the software at MGU Innovation Foundation PARAMASTRA HPC, MG University Campus, Kottayam should be enclosed without any additional cost.
3. Tenders received after the due date will not be considered.
4. Financial bids of those who technically qualified alone will be evaluated.
5. The sample of the product should be approved by the purchasing authority.
6. The rates furnished by bidders shall be inclusive of statutory duties, all taxes, transportation, delivery and installation charges (taxes & Charges has to be clearly shown separately in the Financial Bid).
7. Once the tender has been accepted, the bidder will be liable to supply the products/execute the works to the destinations as per the Purchase/Work Order within the time stipulated for delivery.
8. The items supplied against the tender must strictly conform to the specifications as prescribed in tender. If there is any variation in the specification of the product supplied the same has to be replaced.
9. The assurance of quality, time bound supply, delivery and installation of the products/execution of works at customer site will be the sole responsibility of the bidder and they should ensure the same.
10. The Successful bidder on award of Purchase order based on the tender, has to return a copy of the same to MGU Innovation Hub duly signed and sealed as token of acceptance.
11. Transporting of materials to our customer site will be the responsibility of the supplier and hence the prices shall be inclusive of transportation charges including loading and unloading.
12. The assurance of quality, time bound delivery, supply and installation of the products/execution of works at customer site will be the sole responsibility of the bidder and they should ensure the same.
13. The successful tenderer shall submit the agreement in Rs 200/-stamp paper and within the period specified in the letter of acceptance of his tender/supply order.
14. If the bidder fails to honor the Purchase/Work Order or fails to deliver the products/execution of works in time, the MGU Innovation Hub will make its own arrangement for supplying the products/execution of works at the cost of the bidder. If the Corporation incurs any loss in this account, the amount will be recovered from

the bidder.

15. MGU Innovation Hub or the ultimate customer will be doing a final inspection for the product/work supplied/delivered/installed and shall reject the material at the cost of the supplier in case of quality/specification complaint. The rejected goods are to be removed from supply point at the expense of supplier and materials should be replaced within time limit as intimated by MGU Innovation Hub.
16. The MGU Innovation Hub will in no way indemnify against any eventualities arising out of the low quality of products/work/service and punishments by the legal/statutory authorities due to negligence, wilful act on the part of the bidder or his representative engaged by the bidder. All such issues are to be solved by the bidder at his own risk.
17. Those who have been terminated or blacklisted by Govt. / Kerala/MGU Innovation Hub will not be able to participate in this tender.
18. Samples and specimens have to be provided as per the tender requirement wherever necessary.
19. The following documents are to be presented by the successful bidder for payment after supply: certificate has to be produced from the Customer department with specific remarks.
20. The rate offered must be valid for 60 days.
21. MGU Innovation Hub shall make payment to the successful bidder only after collecting sales proceeds and deducting the service charges. No interest is paid to bidder for belated payments from the customer department.
22. The Earnest Money Deposit will not bear any interest.
23. The Chairman, MGU Innovation Hub reserves the right to accept or reject the tender/tenders without assigning any reason thereof.
24. For further details contact MGU Innovation Hub, MG University Campus, Athirampuzha, Kottayam, Phone no. 8078010009

ELIGIBILITY CRITERIA

1	Bidder should be, a Company registered in India	Copy of valid Registration certificates / Copy of Certificates of incorporation
2	Cumulative Turnover shall be a minimum of an average 1Cr. in last 3 financial years.	CA certified Balance sheet proof to be attached.
3	Should not have been blacklisted by any of the Government entities under state / central Govt.	Self-Certificated
4	The bidder should have a registered number of 1. GST where his business is located 2. Income tax / PAN number	Copies of relevant certificates of registration
5	The bidder should have a valid certificate issued by any Govt. of India Enterprise.	Documentary proof
6	The Bidder should submit a Manufacturer Authorization Form (MAF) from the OEM for all the quoted products along with the technical bid	MAF
7	Bidder should have experience of having successfully completed similar projects.	Work orders to be attached

- 1) The intended bidders can verify the proposed site and building (MGU Innovation Foundation building) between 10.15 am and 4.45 pm on all working days till the last date of submission of tender.
- 2) The quoted price in the BOQ should be inclusive of all taxes, freight, loading & unloading/installation charges.
- 3) Details such as make, model, mode of operation, etc., should be clearly mentioned in the quotation.
- 4) Quoted rates should have at least two two-month validity period.
- 5) The right to accept or reject the quotations without assigning any reason rests entirely with the undersigned.
- 6) The tender should be of branded quality products
- 7) Brochure of products and different models quoted should be closed.

- 8) If a negotiation meeting is convened by the undersigned, the authorized person of the firm should attend the meeting in time at their cost.
- 9) The payment process will be initiated only after a satisfactory supply of the items and installation after receiving reports from the experts from the MGU Innovation Foundation.
- 10) If the date of receipt and opening of the tenders is declared a holiday, the same time of the next working day will be the last date and time for the purpose.

The bids shall be opened at the date and time specified. Further details can be had from the MGU Innovation Foundation, Mahatma Gandhi University, Kottayam, Kerala-686560 on all working days during working hours. Phone no. Mob: 09778429535(CTO, MGUIF) 8078010009 (Purchase, MGUIF). The bidders are advised to submit their bids well in advance to avoid any kind of network problems. The under-signed reserves the right to reject any or all of the tenders without assigning any reason whatsoever

Sd/-

**Chairman & Managing Director
MGU Innovation Foundation**