



Ref. No.: SMVDU/PM-USHA/SoP/25/588

Dated: 30/01/2025

Notice Inviting Quotation

Sub:- Supply of NANODCAL-RESCU Software

Quotations in sealed cover are invited for the supply of **Supply of NANODCAL-RESCU Software** on behalf of Registrar SMVDU for the Head, School of Physics, SMVDU; from reputed registered firms having a valid GST Number and PAN Number, and for supplying rates for the below mentioned jobs:

S. No.	Name of the Item	Detailed Specifications	Qty
1	NANODCAL - RESCU Software	<p>1. Software should be able to predict the electronic structure and derived properties of bulk materials, material surfaces and molecules using density functional theory (DFT) and DFPT (perturbation theory) solver. It should calculate the ground-state density using a basis of numerical atomic orbitals, plane-waves or real space grids, or a combination of them.</p> <p>2. Software should be state-of-the-art DFPT implementation that should allow the users to compute useful physical parameters like the dielectric tensor and the dynamical matrix, phonon spectra, as well as response functions like the dielectric permittivity using Rescu tool.</p> <p>3. Software should have following key features:-</p> <ul style="list-style-type: none"> · Solve small and large scale systems/ · DFPT – Response functions · DFT + EXX (hybrid) (Hartree-Fock method) · DFT + U (Hubbard model) · Spintronics (collinear / non-collinear / SOC) · Density of States (DOS, PDOS, LDOS, PLDOS) · Raman properties, Optical properties · Electronic & band structures calculation and analysis tools · Phonon tools (finite-difference-based) · Wannier functions calculator & Band-unfolding · Berry curvature calculator (for topological properties). <p>Specification of Nanoscale material & device Simulation Tool (DFT+NEGF)</p> <ul style="list-style-type: none"> • Numerical Simulation Engine features Should support following below feature: • Density Functional theory with Non Equilibrium Green Function (NEGF – Quantum Transport) feature. • Predicts quantum electronic structure and transport properties in nanoscale devices from first principles using Nanodcal tool. • Computes the properties of atomic arrangement (molecules, crystals, surfaces & device) from first principles using density functional theory (DFT+ NEGF). 	01

Signature

- Calculate nonlinear and non-equilibrium quantum transport properties up to 6 probe device structures with following features below.
- Molecular electronics (small to large scale systems atoms)
- Spintronics (collinear / non-collinear / Spin-Orbit Coupling)
- Semiconductor nanoelectronics (I-V curve)
- Nano-wires, Carbon nanostructures
- Metal contacts and interfaces etc.

Graphical User Interface (GUI) Features for building the structure:

- Device Studio graphical user interface for modeling with following parameter.
 - Crystal structure builder to define Lattice parameters, space group etc
 - Molecule modeling, Material Interface builder.
 - 6 probe Device Structure builder.
 - Surface modeling, Nanowire Nanotube, Nanoribbon.
 - Supercell modeling, Grain Boundary
 - 2 & 3 Terminal (FET) Device Modeling.
- Software can bend the left & right (both) side of device electrode on given angle.
- Software is able to define & calculate following DFT parameters.
 - Basic (Electron Temp, Energy cut-off, Exchange correlation, K-Point
 - Contour integral (Integral lower bound, Circle point)
 - Electrode parameter (Electron temperature, Electrode Voltage, K point)
 - Iteration control (Density Matrix, Hamiltonian matrix, Realspace density)
 - Basis Set (LDA, PBE, Single zeta polarized and Double Zeta polarised)
 - Spin type (No Spin, Collinear Spin, General Spin, Spin- orbit interaction)

Software can calculate following material & device output properties.

- Density of State, Effective potential.
- Total energy, Bandstructure, Charge, Hessian, Phonon Bandstructure.
- Electron Density, Potential, Transchennel.
- Eigen State, Full band structure, Effective Mass.
- Complex Bandstrucure, ZT, Phonon Density of state,
- Phonon full band structure, Phonon Transchannel, Modulus.
- Scattering State, Transmission, Photo current, IV Curve
- Conductance, Thermoelectric current, Seebeck coefficient etc.

***Only OEM or authorised reseller must quote**

The sealed rate quotations should reach the Central Dispatch Section SMVDU latest by 10/02/2025, by 2:30 P.M. Any quotation received after the due date and time shall be summarily rejected. The sealed bids shall be opened on the next working day at 2:30 P.M. in the presence of authorized representatives, should they wish to attend the same.

Terms & Conditions

1. Rates should be written in figures as well as words. Delivery duration. GST rates. Delivery charges or any other rates/charges, as applicable, and discount if any, should be clearly mentioned in the **Schedule of Quantities** [Format enclosed at Annexure 'A'].
2. **The last date for receipt of sealed quotations in the Central Dispatch Section SMVDU is latest by 10/09/2025 at 2:30 P.M.**
3. The quotation / **Schedule of Quantities** should be on the letter head of the Company with reference no. and date on it duly signed and stamped.
4. The quotations should be submitted in sealed cover, addressed to the Head of School of Physics, super-scribing the NIQ issue number & date and due date & time failing which the quotation is liable to be rejected.
5. Price quoted for the material / equipment/ service as may be applicable shall be final and valid for 3 months.
6. Quotation without the authorization from the Company will not be accepted.
7. Delivery of material /equipment / service as applicable mentioned in this quotation will be supplied/ provided by the supplier at School of Physics, SMVDU, Kakryal, Katra-182320 (J&K).
8. Rate offered must be for a metric system of unit lengths or volume or weight in case of procurement of material/ items.
9. Documents in support of valid GST and PAN Number also need to be enclosed with the quotation.
10. SMVDU reserves the right to increase the quantity mentioned in this NIQ or to split this quotation and place order on one or more suppliers/ bidders; as well as, the right to reject partly or completely, the quotations without assigning any reasons thereof in case of procurement.
11. The quotation should be complete in all respects and the firms shall give the Make/ Brand name offered for the items/ spare parts in the quotations. Wherever applicable, technical literature may please be enclosed along with quotation.
12. The payment shall be released only after the receipt of all and complete material/equipment/ service (equipment/ items) having being brought back to good working condition and its inspection by a duly constituted Inspection Committee.
13. Material/ equipment shall be guaranteed/warranted for the minimum period of 01 year on site for satisfactory performance, workmanship and for the quality of material/ equipment supplied by the firm from the date of delivery/ installation.
14. Quotation received after DUE DATE & TIME will not be considered. SMVDU shall not be responsible for delays in postal transit.
15. All taxes / duties should be clearly mentioned in the Quotation.
16. In case of service the authorized vendor/ service provider shall mention detailed heads of expenditure which shall include inter area cost of spare parts, visit of service engineer, postal charges if any, cost of shifting the equipment/ item to the service centre and back if any etc.
17. **PACKING:** The equipments shall be packed suitably for dispatch directly to SMVDU at Suppliers expenses and supplier shall be responsible for any damage during transit.



18. AFTER SALES SERVICE: The offer shall clearly state full details of the after sales service facility available for the equipment.
19. JURISDICTIONS FOR DISPUTES: In all disputes, the decision of the Registrar, SMVDU, shall be final, conclusive and binding on the supplier. All disputes shall be subject to the jurisdiction of the courts in the District, Jammu.
20. DEVIATIONS: Deviations, if any from the specifications given which provide for improvement in the functioning of the equipments will be accepted. Such deviations and their advantages shall be clearly brought out in the tender / quotation.
21. **The vendor must attach a certificate by the OEM on their letterhead stating that the above software is their proprietary item.**
22. **The vendor must attach an authorization certificate by the OEM on their letterhead authorising the vendor submitting the quote as the authorized sole reseller of the said software in India.**
23. **Any quotation received without the above certificate shall be outrightly rejected.**
24. **Five Years Technical support (updates and reinstallation in case of System change due to hardware crash or any other reasons).**

The NIQ shall be available on the University Website: www.smvdu.ac.in. For any query contact School of Physics, SMVDU at the following email id: office.sop@smvdu.ac.in

Signatures:.....

Head, School of Physics

Date: 30-01-2025

[Handwritten signature]

[To be provided on Firm/Company Letter Head]

Schedule of Quantities

Name of the Job: Supply of NANDCAL-RESCU Software

Ref: NIQ Number :..... Date:

Sr. No.	Details of the Item	Qty.	Rate per item	Amount in Rs.	GST rate	GST Amount in Rs.	Total Amount inclusive of GST in Rs.
1							
	Less: Discount if any						
	Add: Delivery Charges if any						
	Net Amount to be paid in Rs.						
	Delivery Period						

Additional Terms and Conditions [if any]:

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Bank details for RTGS Transfer

Name of the Account:

Account No.:

Account Type:

Bank Name:

Branch name and Address:

IFSC Code:

Signature & Stamp of the Supplier

