D No. 563 /APD
Date 3-10-19

ENQUIRY FORM

DEPARTMENT OF APPLIED PHYSICS

Z. H. College of Engg. & Tech., A.M.U. ALIGARH

Dated: 03/10/2019

Ref. No. APD-01/2019-20/Virtual Nano-lab from Synopsys Quantum wise Inc:

M/s_____

Please quote your lowest rates allowing concessions given to Academic Institutions, if any, for the following articles, illustrations/specification, stating delivery time, should be given in each case. Quotation under sealed cover bearing the **Ref. no.** should reach this office on or **before 21/10/2019 by 3:00PM.**

S.No	Particulars
1	**Synopsys QuantumATK for Nanotechnology Simulation – Academic Bundle – Materials Only.** 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 semi-core 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 300 bond-order potentials included. 2.1.2. Two/three-body potentials: Lennard-Jones (various versions), Coulomb (various versions), Stillinger-Weber, 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.