	INDIAN INSTITUTE OF TECHNOLOGY BOMBAY **MATERIALS MANAGEMENT DIVISION** **Powai, Mumbai 400076.**

Ref No.(PR No. 1000050693) **(Rfx No. 6100002458)**

Technical Specifications : BIOVIA Material Studio Academic Research
(Qty : 2)

Sr. No	Item Description	Detailed Technical Specification	Technical Compliance (Yes / No)	Additional Information (if any)
1	**BIOVIA Material Studio Academic Research**			
1.1	Materials Studio 3D Visualizer: Polymer builder Nanostructure builder Analog builder Transport device builder Mesostructure builder Crystal builder Surface builder Layer builder	A graphical user environment-in which user can construct, manipulate and view models of molecules, crystalline materials, surfaces, polymers, and mesoscale structures. This is to be complemented by a complete set of solution methods including quantum, atomistic, classical, mesoscale, and statistical that enable user to evaluate materials at various particle sizes and time scales. The software should allow user to easily build, modify, visualize and simulate a wide range of materials including molecular and inorganic crystals with following simulation capabilities: • Easily build and visualize many different material types from organometallic complexes to polymers, crystals, surfaces, and catalysts. • Identify compounds with optimal physicochemical properties for Quantitative		

		Structure-Activity Relationships and extend the base tools to include a neural networks model building method and accurate quantum mechanical descriptors.		
1.2	BOVIA Material Studio Research suite with perpetual license option	The software is required to provide a complete modelling and simulation environment which enable the researcher to predict and understand the relationships of atomic / molecular structure of a material with its properties and behaviour. The software must consist of a wide variety of robust computational modules conforming to quantum, classical, mesoscale, analytical, statistical and visualization tools as described below		
1.3	BIOVIA Materials Studio CANTERA	Should be able to generate chemical rate equations. It should provide environment for configuring the thermodynamic input, and for executing these calculations. Cantera Reaction Editor should enable users to introduce new species and reactions, optionally with reaction rates determined from Materials Studio DMol3, into complex reaction schemes with existing experimentally determined thermodynamic data. The software connects the quantum chemical reactions to CSTR, PFD, TPD analytical calculations.		
1.4	BIOVIA Materials Studio CASTEP	Materials Studio CASTEP simulates the properties of solids, interfaces, and surfaces for a wide range of materials including ceramics, semiconductors, and metals using a plane-wave density functional method.		
1.5	BIOVIA Materials Studio DMol3	DMol3 is used to model the electronic structure and properties of organic and inorganic molecules, molecular crystals, covalent solids, metallic solids, and infinite surfaces using DFT. DMol3 uses numerical basis sets as basis rather than Gaussian basis. This description allows for better quality orbitals, minimized BSSE correction and better description for weak bonds. Localized basis calculations are enabled for both periodic and non-periodic		

		DFT. The Effective Screening Medium (ESM) option in DMol3 replaces the periodic boundary condition along the z-direction with a screening medium, such as a vacuum or metal, at the cell boundary. It should calculate reaction pathways, including minimum energy pathways, transition states, multi-step reactions using a unique Hybrid Eigenvector-Following and Doubly Nudged Elastic Band Method for Finding Transition States.		
1.6	BIOVIA Materials Studio DFTB+	Materials Studio DFTB+ is a semi-empirical module for simulating electronic properties of materials. It uses a tight binding approach based on density functional theory to enable quantum mechanical accuracy on larger system size. It should calculate reaction pathways, including minimum energy pathways, transition states, multi-step reactions using a unique Hybrid Eigenvector-Following and Doubly Nudged Elastic Band Method for Finding Transition States.		
1.7	BIOVIA Materials Studio KINETIX	BIOVIA Materials Studio KINETIX is a general-purpose program for simulating the competing chemical and physical adsorption, desorption and diffusion processes taking place at surfaces. This should provide unique insights such as the role of species diffusion in catalyst activity and poisoning, and surface coverage of species at up to microscales. A program for the simulation of chemical and physical processes taking place at crystal surfaces using kinetic Monte Carlo methods (KMC).		
1.8	BIOVIA Materials Studio ONETEP	Materials Studio ONETEP is a linear scaling DFT code, enabling accurate, first principles calculations on systems of up to thousands of atoms. The grand-canonical ensemble in ONETEP is useful for simulating systems with a variable number of electrons and a fixed external potential. It should be able to run up to		

		10000+ cores CPUs for large scale system linear DFT calculation.		
1.9	BIOVIA Materials Studio QMERA	Materials Studio QMERA employs QM/MM method combining the accuracy of a quantum with the speed of a forcefield calculation. This approach should make it possible to perform accurate calculations on very large systems for substantially less effort.		
1.10	BIOVIA Materials Studio VAMP	Materials Studio VAMP is capable of rapidly predicting many physical and chemical properties for molecular organic and inorganic systems using a semi-empirical molecular orbital method. Materials Studio VAMP is an ideal intermediate approach between forcefield and first principles methods.		
1.11	Plug-in to Gaussian software	Access Gaussian's broad range of ab initio modeling methods via the easy-to-use graphical interface.		
1.12	BIOVIA Materials Studio Adsorption Locator	Materials Studio Adsorption Locator finds low-energy adsorption sites for molecules on both periodic and non-periodic substrates		
1.13	BIOVIA Materials Studio Amorphous Cell	Should allow to construct representative models of complex amorphous systems constituting small molecules, metallic and non-metallic interfaces, polymers and ceramics using Monte Carlo based algorithms.		
1.14	BIOVIA Materials Studio Blends	Predicts phase diagrams and interaction parameters for liquid-liquid, polymer-polymer, and polymer additive mixtures, phase equilibria, and separations technology.		
1.15	BIOVIA Materials Studio Conformers	Provides conformational search algorithms and analysis tools to characterize molecular conformation and flexibility. The search method should include Random sampling, systematic grid scan method, Boltzmann jump method and should allow to analyse various properties such as RDF, RMSD, RoG etc.		
1.16	BIOVIA Materials Studio Forcite and Forcite Plus	It offers molecular mechanics and dynamics methods for molecules and periodic systems. The tool includes a wide range of analysis		

		features to predict mechanical properties, diffusivity, local structure, density variations, cohesive energy density, dipole autocorrelation functional and more. Supported forcefields are Materials Studio COMPASSIII, CVFF, PCFF, Dreiding, and Universal. Can perform reactions in MS Forcite classical module by referring to transition state calculations created in MS DMol3. This table is referred during molecular dynamics to perform reaction MD via MC-MD method implemented as MS Reaction Finder script. Machine Learning Interface Potentials (Force fields) using message passing or multiatomic cluster expansion (MACE) potential for simulations. MACE is an architecture for machine-learned potentials for atomic simulation. MACE-OFF23 with closed shell organic molecules. MACE-MP0b with inorganic materials. It also supports execution on GPUs for accelerated performance.		
1.17	BIOVIA Materials Studio GULP	GULP is a method for optimization, property calculation and dynamics of materials. It allows to utilize the GULP ReaxFF library, ReaxFF SEI2021, for modeling the surface-electrolyte interphase. Additionally, it allows to calculate properties for variable charge models, including charge derivatives for electric fields. This enhancement enables GULP ReaxFF calculations with electric fields.		
1.18	BIOVIA Materials Studio Sorption	Sorption provides a means of predicting fundamental properties needed for investigating adsorption and separations		

		phenomena, such as sorption isotherms and Henry's constants.		
1.19	BIOVIA Materials Studio Mesocite	Mesocite is a coarse-grained simulation module for the study of materials at length scales ranging from nanometers to micrometers and time scales from nanoseconds to microseconds. Materials Studio Mesocite can provide structural and dynamic properties of fluids in equilibrium, under shear or in confined geometries. Granular Molecular Dynamics: Study the formation of structures at the scale of particle grains and simulate how those structures change during manufacturing steps. One can utilize the Granular Dynamics task in Mesocite to simulate the motion of particles with negligible thermal velocity, predicting the arrangement of mixed particle systems. Supported force fields include Shinoda, MS Martini3 with elaborate tools for Coarse graining molecules to beads for both preprocessing and post processing tasks.		
1.20	BIOVIA Materials Studio MesoDyn	MesoDyn is a classical density functional method for studying the long length- and time-scale behaviour of complex fluid systems, in particular the phase separation and structure of complex polymer systems.		
1.21	BIOVIA Materials Studio Morphology	It allows to predict crystal morphology from the atomic structure of a crystal. Morphology allows for the prediction of crystal shape, the analysis of crystal surface stability, the development of tailor-made additives, and the control of solvent and impurity effects.		
1.22	BIOVIA Materials Studio Polymorph Predictor	Polymorph Predictor has been developed for use with fairly rigid, non-ionic or ionic molecules composed primarily of carbon, nitrogen, oxygen, and hydrogen. The approach is based on the generation of possible packing arrangements in all reasonable space groups to		

		search for the low-lying minima in lattice energy.		
1.23	BIOVIA Materials Studio Reflex: Reflex Plus Pattern Processing Powder Diffraction Powder Indexing Powder Refinement Powder Quantitative Phase Analysis (QPA) Powder Solve	**Reflex simulates X-ray, neutron, and electron powder diffraction patterns based on models of crystalline materials. Reflex Plus offers a complete package for the determination of crystal structures from medium- to high-quality powder diffraction data.** **Reflex QPA extends the Reflex functionality for quantitative phase analysis, allowing for the determination of the relative proportion of different phases, including both inorganic as well as organic systems, in a mixture based on powder diffraction data.** **Direct space methods for solving crystal structures from X-ray (or neutron) powder diffraction data involve generating a large number of trial crystal structures in direct space and finding the solution that minimizes the figure of merit.** **Powder Solve uses a combined figure of merit. This combines information from the experimental diffraction pattern, in the form of the Rwp measure of similarity, with an energetic contribution which accounts for the fact that possible structure solutions should be free of close contacts between structural fragments.** **Powder Refinement for performing modified Pawley or Rietveld refinement of crystal structures against experimental data and for joint optimization to match experimental powder patterns while simultaneously minimizing the potential energy.**		

1.24	BIOVIA Materials Studio QSAR and QSAR Plus	QSAR's (Quantitative Structure-Activity / property Relationships) integration in Materials Studio provides access to a wide range of descriptors and advanced analysis capabilities to help generate high quality structure activity / property relationships. QSAR includes a wide range of descriptors including topological and electro-topological descriptors. Also, Jurs descriptors enable charge distribution on solvent surfaces to be examined; VAMP Descriptors further extend the range of 3D descriptors into those including electronic interactions; and GFA applies a sophisticated genetic algorithm method to calculate quantitative structure-activity / property relationships.		
1.25	BIOVIA Materials Studio Synthia	Synthia calculates properties of homo- and copolymers using advanced Quantitative Structure-Property Relationships (QSPRs). It allows researchers to rapidly screen candidate polymers for a wide range of properties.		
1.26	Documentation	Software comes with in-detail theory covering the concepts of computational materials modelling and include tutorial examples to understand software operation.		
1.27	Warranty of the system			1 year