Technical Specification:

2	1	A Software which provides a complete modelling, simulation and visualization environment **which enables the researcher** to predict and understand the relationships of atomic / molecular structure of a material with its properties and behaviour.	• Nature of license should be perpetual • Supplier should provide 12 months warranty from the date of generation of License • Supplier should provide an entitlement to purchaser for software upgrade, trouble shooting and maintenance during warranty period • Vendor should have supplied this software to at least 2 IITs (Indian Institute of Technology). User certificate should be provided. • Vendor should optionally quote for additional warranty and technical support DETAILED SOFTWARE SPECIFICATIONS The software must consists of a wide variety of robust computational modules conforming to **quantum, classical, mesoscale, analytical, statistical and visualization tools available in different bundles, the specifications of each bundle is detailed below.** **BUNDLE-1 Quantum Mechanical tools** Validated and efficient quantum mechanical applications based on Density Functional Theory (DFT), hybrid QM/MM and semi-empirical methods. Quantum mechanical methods should yield accurate thermodynamic, kinetic and structural results, providing an efficient input to experiments and also provide insights into processes at the atomic level. It should accurately predict molecular and crystal geometry, chemical reaction pathways, optical properties, spectra (IR, Raman, NMR, EELS, ELNES, XES, XANES, EXAFS etc). The quantum mechanical tools should consists of different modules with following simulation capabilities: ▪ It should offer simulation capabilities such as accurate prediction of phonon spectra, dielectric constants, and optical properties. It should simulate the	

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			properties of solids, interfaces, and surfaces for a wide range of materials classes, including ceramics, semiconductors, and metals, with a fast density functional theory (DFT) quantum mechanical code and also include an improved implementation of the Density Functional based Tight Binding (DFTB) quantum simulation method for the study of electronic properties of materials containing hundreds of atoms. ▪ It should combine computational speed with the accuracy of quantum mechanical methods to predict materials properties reliably and quickly. ▪ It should have access Gaussian's broad range of *ab initio* modelling methods via the easy-to-use graphical interface. ▪ It should predict NMR chemical shift tensors, isotropic shifts, and electric field gradients for any material ▪ Accurately treat systems such as grain boundaries, nanoclusters and protein-ligand complexes with the quantum mechanics-based program designed specifically for calculations on large systems of more than 500 atoms. ▪ It should combine the accuracy of quantum mechanics with the speed of a force field calculation to perform calculations on very large systems in a cost and time effective manner. ▪ It should predict fundamental properties, such as sorption isotherms and Henry's constants needed for investigating separations phenomena. It must also be able to find the most stable adsorption sites for a broad range of materials. ▪ It must have capability to rapidly calculate physical and chemical properties of molecular organic and inorganic systems ▪ It must include a solver for chemical rate equations. Given the starting composition of a mixture of reactants, it should be able to predict the outcome of the reaction in terms of the composition of the product mixture **<u>Bundle-2: Classical Simulation tools</u>** This bundle must construct and characterize models of isolated chains, crystalline and amorphous bulk materials. It should be	

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			capable of predicting key properties like miscibility and blending, cohesion and wetting, mechanical behaviours, diffusion, and adhesion at surfaces. The classical simulation tools should consists of different modules with following simulation capabilities: ▪ The module should be able to provide an understanding of molecular properties and behaviour, especially for liquids and amorphous polymers with versatile computational tools. It should predict and have tools to investigate properties such as cohesive energy, density, equation-of-state behaviours, chain packing and localized chain motions. ▪ It should also predict phase diagrams and interaction parameters for liquid-liquid, polymer-polymer, and polymer-additive mixtures to study the structural factors affecting the behaviour of blends and formulations. ▪ Simultaneously and accurately predict structural, conformational, vibrational, and thermophysical properties for a broad range of molecules in isolation and condensed phases under a wide range of temperature and pressure. ▪ It should be able to characterize molecular conformation and flexibility, provide insight into geometric and energetic properties and probe geometry-property relationships, which have application in many fields including crystallization, catalysis, and polymer studies ▪ It must be capable of quickly perform reliable geometry optimization of molecules and periodic systems and fast energy calculations and extend this to include molecular dynamics, dynamics protocols and analysis tools. ▪ It must extend the range of materials and properties that can be studied with a wide range of materials force fields, from shell models for ionic systems to embedded atoms for metals to molecular mechanics force field support for covalent systems. ▪ It must have the capability to allow the study of mesoscale structured materials using coarse grained molecular dynamics	

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			and dissipative particle dynamics (DPD). ▪ Capabilities to study the dynamic nature of mesoscale structures, including polymer melts and blends should also exist. ▪ It must predict the bulk properties of multi-component, nano- structured materials systems with this standalone product. ▪ Allow calculation of polymer properties using advanced Quantitative Structure-Property Relationships (QSPRs) allowing for rapidly screened candidate polymers for a wide range of properties as well as property prediction of copolymer blends. ▪ It must include a program for the simulation of chemical and physical processes taking place at crystal surfaces using kinetic Monte Carlo methods, KMC **<u>Bundle-3: Analytical and Crystallization tools</u>** The analytical and crystallization module should help investigate, predict, and modify crystal structure and crystal growth. It must simulate particle morphology, predict crystal structure and provide an understanding of polymorphism, study surface interactions, and design growth-mediating additives. The analytical and crystallization tools should consists of different modules with following simulation capabilities: ▪ Predict crystal morphology from the atomic structure of a crystal, develop tailor-made additives and control solvent and impurity effects. ▪ Ability to analyse connectivity information, categorize and score proposed structures. ▪ Predict potential polymorphs of a given compound from the molecular structure and study fairly rigid, ionic and non-ionic molecules. ▪ Simulate X-ray, neutron and electron powder diffraction, determine crystal structure, assist the interpretation of diffraction data and validate the results of experiments and computation. ▪ Determination of crystal structures from medium- to high-quality powder diffraction data.	

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			▪ Determine the relative proportion of different phases in a mixture of inorganic/organic systems based on powder diffraction data. ▪ Obtain quality powder diffraction data from X-ray, neutron and electron radiation sources using a novel and robust indexing algorithm. **<u>Bundle 4: Visualization and Statistics tools</u>** 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 materials 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.	