MATERIAL SCIENCE SUITE WORKSHOP

28th – 30th September 2017

International Medical University, Kuala Lumpur, Malaysia

	Day 1 Organic molecules, organometallic complexes and crystals: Model building with Quantum Mechanics (QM) calculations	**Day 2** Organic and inorganic molecules, nanostructures, nanoparticles, polymers, copolymers and dendrimers: Model building with Molecular Dynamics (MD) simulation and analysis	**Day 3** Application of simulation to research project/industry
Morning session	• Introduction • Model building: - Organic molecules - Organometallic complexes - Combinatorial libraries - Crystal builder	• Model building: - Building complicated organic/inorganic molecules, - Building nanostructures and nanoparticles - Building linear and branched polymers, copolymers and dendrimers - Conformational search - Disordered system builder - Interface builder	• QM and MD application examples: - Spin state and binding energy - Hole mobility calculation - Crosslinking polymers - Thermophysical properties (Glass transition temperature) - Possible addition/substitution on Probe Grid scan and/or Quantum ESPRESSO
Lunch Break			
Afternoon session	• QM calculations - Density functional theory (DFT) and semiempirical QM modelling - Single point energy and optimization calculation (Basis sets and functionals) - Properties calculations(Vibrational properties, IR spectrum, electrostatic potential, molecular orbitals, partial charges, optical properties) - Transition state search - Time-dependent DFT	• Applications of MD - MD simulation - Multistage simulation workflow - MD analysis (Volume, density, solubility and pressure tensor) - Diffusion coefficient - Radial distribution function	• How simulations can be applied to my research project/industry?