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Molecular Dynamics Simulations of Interfaces in Complex Materials

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Molecular details of structure and chemistry play and important role in the properties and engineering performance of composites and complex materials. Experimental investigation of the interfaces most often presents itself as a major challenge. This, in turn, becomes an opportunity in disguise for the molecular level simulation approaches. However, in order to convincingly address to the problem of elucidating the structure and chemistry at the interfaces, one must employ reliable and accurate and transferrable interaction potentials for dissimilar materials - this is the case for composites and complex materials. In this, talk we will present examples of molecular dynamics studies on the structure and properties of silicon nano-crystals in a silica matrix, piezoelectric CNT-polyimide nano-composites, and on the role of super lattice structures for enhancing mechano-electric coupling in ferro-electric ceramic alloys.