

Seminar

Concept of Density and Materials Modeling at Different Length Scales

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One of the concepts that has played a major role in the conceptual as well as computational developments covering all the length scales of interest in a number of areas of chemistry, physics and materials science is the concept of single-particle density. This encompasses the (i) electron density in the short (microscopic) length scale, (ii) particle number density in the intermediate (mesoscopic) length scale and (iii) property density in the large (macroscopic) length scale that considers materials as a continuous medium. In spite of the differences in the nature of the density variables used in different length scales, the corresponding theoretical frameworks involving energy density functional have been found to possess an underlying unified structure, covering quantum as well as classical systems. Within this broad framework, theoretical and computational design of molecules and materials for specific applications, has attracted a great deal of attention in recent years. Our humble contribution to the formalism of density based modeling at different length scales and application to hydrogen energy related issues of generation and storage of hydrogen as well as structure and dynamics of soft matter will form the subject matter of the talk.

Friday, Nov 8th 2019

2:00 PM (Tea/Coffee at 1:30 PM)

Auditorium, TIFR-H