TIFR Centre for Interdisciplinary Sciences, Narsingi, Hyderabad 500075

Seminar

Computational Studies: From Clusters to Catalysis

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Abstract: The primary focus of my research is on the application of computational chemistry to understand problems of general interests. This spans two different research areas, namely, the design of novel nano materials and delineating catalytic reaction mechanisms. During the first part of my presentation, I will focus on the application of computational chemistry on the design of boron and lithium doped germanium clusters. In the second part of my presentation, I will discuss specific examples on the application of density functional theory in understanding catalytic reaction mechanisms and the importance of interplay between theory and experiment.

***Date*: Thursday, February 21st 2013**

***Time*: 02:30PM (Tea/Coffee at 02:15PM)**

***Venue*: Conference Hall, TCIS**

All are cordially invited