Laboratoire des Solides Irradiés, UMR 7642

Séminaire – Lundi 10 mars 2014 (10:30)

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Salle du laboratoire PMC (05-3029A)

10H00

Phase transitions under pressure,
thermal transport and excitons dispersion : a multi-scale journey.

In this talk, I will review topics and methodologies I have studied during my Phd at King's College London and my first postdocs at Paris 6 and EPFL. I will then present the project I am currently working on here at LSI. In my PhD, I have focussed on understanding the microscopic mechanisms of structural transformations using atomistic simulation techniques. I will present a method, namely the Metadynamics, for accelerating rare events and sampling the free energy. I will then show how by using this method I studied several "rare events" such as phase transitions in CdSe and Si nanocrystals under pressure, structural transformations in green tea catechins and their interaction with the cardiac protein troponin C. Moving then to the topic of my first post docs, I will speak about the first principles theoretical approach I developed for evaluating the lattice thermal conductivity by exactly solving the Boltzmann Transport Equation. I will review the major results obtained for 3D and 2D semiconductors materials and how the dimensionality, the strain and the isotopic enrichment affect the thermal response. Finally, I will present the subject of my research here at LSI. By using a recent scheme for calculating exciton dispersions, based on the first-principles many-body Bethe-Salpeter equation, I start studying the properties of layered materials. I will present the preliminary results obtained for hexagonal BN and the good agreement with inelastic x-ray scattering results present in literature.