Dipartimento di Fisica e Astronomia Galileo Galilei

Università degli Studi di Padova

AVVISO DI SEMINARIO

Seminari di Fisica Statistica e Teoria della Materia Condensata

Giovedì 22 gennaio 2015
ore 15:00
Aula R

Dr. Marcelo A. Carignano

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"$CH_3NH_3PbI_3$ perovskite: A first principles molecular dynamics study"

Hybrid organic-inorganic perovskites have attracted the attention of the photovoltaic research community during the past five years due to their promising performance as light harvesting material. In particular, $CH_3NH_3PbI_3$ is the prototypical example on which most of the experimental work has been done and the system that we have selected to perform this computational study consisting of a molecular dynamics simulation based on forces calculated from density functional theory. Two different system sizes have been considered, one with 8 unit cells (384 atoms) and a larger one with 27 unit cells (1296 atoms) and the simulated time reaches 40 ps. Our findings, obtained using the CP2K software package, reveal the interplay between the thermal energy of the system and the electronic degrees of freedom. For example, the organic molecule undergoes relatively fast rotations and the energy band gap (approximated by the LUMO-HOMO energy difference) fluctuates around the equilibrium value of ~1.5 eV with a width of 0.2 eV. Our study also provides a quantitative measure for the finite size effects affecting the calculated properties and provides a contextual scenario on which to analyze the more typical density functional theory studies based on static calculations on optimal structures.

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