Simulating energy conversion processes from first principles

Giulia Galli

Institute for Molecular Engineering
Department of Chemistry
The University of Chicago, Chicago, Il, USA
Email:gagalli@uchicago.edu

We describe recent progress in describing heterogeneous, defective materials with complicated morphologies using first principles methods, including electronic structure calculations and ab initio molecular dynamics. We focus on two examples: interfaces for solar energy conversion processes, and materials composed of complex building blocks, e.g. assemblies of nanoparticles used in colloidal solar cells. We aim at showing the importance of unraveling mechanisms and providing fundamental, physical insights, in order to pave the way to material design strategies.