

Next-Generation Pb-free Photovoltaics: All-inorganic Perovskite to Kesterite

Vijay Singh, Ambroise van Roekeghem, and Natalio Mingo

CEA-Liten, Grenoble, France

Vijay.singh@cea.fr

Photovoltaic (PV) systems, which convert sunlight into either electrical or chemical energy, constitute a promising renewable energy source. Current state-of-the-art PV systems based on perovskites -typically metal-organic halides- have reached impressive performance with record efficiencies rising from 4% to 22% in less than a decade. But most perovskites contain lead, raising environmental concerns, and questions regarding the materials' long-term stability also remain. This is indeed a big hurdle to commercialize these perovskites. In this talk, I will discuss the atomic and electronic structure of *Pb-free* all-inorganic perovskite and kesterites materials for next-generation PV applications. I will also discuss our machine learning model to predict the stability of 1568 kesterites. To elucidate the electronic, magnetic, optical and chemical bonding properties of these materials, we have employed first-principles density functional theory. The phononic properties (i.e. lattice dynamics) were investigated using first principles density functional perturbation theory and a direct, supercell force-constant approach. To treat anharmonic effects beyond perturbation theory, we have used our inhouse code. This talk will illustrate how theoretical results can highlight physical materials properties that might be important for the development of the next generation PV materials.