

MAR16-2015-009468

Abstract for an Invited Paper
for the MAR16 Meeting of
the American Physical Society

Computational design of inorganic-organic hybrid materials energy storage and conversion

ALEXIE KOLPAK, Massachusetts Inst of Tech-MIT

Hybrid inorganic-organic materials are of interest for the design of new functional materials that combine the advantages of both organic and inorganic components to optimize properties and/or obtain new physical phenomena. In this talk, I will discuss our recent work using first-principles density functional theory to design nanostructured hybrid materials for energy storage and conversion applications. In particular, I will discuss the electronic, optical, thermal, and mechanical properties of a class of nanostructured hybrid materials based on layered transition metal phosphates, showing that these materials offer a highly tunable platform for the design of efficient, flexible photovoltaics and thermoelectrics. In addition to optimizing individual properties, I will also discuss exciting possibilities for using this platform for the design of materials with strong coupling between functionalities.