Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Computational Discovery of Two Lead Free Halide Double Perovskites with Band Gaps in the Visible Range: Cs2BiAgCl6 and Cs2BiAgBr6[1] MARINA FILIP, GEORGE VOLONAKIS, University of Oxford, Department of Materials, AMIR ABBAS HAGHIGHIRAD, SAMUEL HILLMAN, NOBUYA SAKAI, BERNARD WENGER, HENRY SNAITH, University of Oxford, Department of Physics, FELICIANO GIUSTINO, University of Oxford, Department of Materials — The perovskite solar cell is emerging as one of the most promising solution processable photovoltaic technologies, with an efficiency that now exceeds the performance of thin-film silicon devices. This performance is exclusively due to the optimum optoelectronic properties of the prototypical methylammonium lead-iodide perovskite (MAPI). However, the presence of lead in MAPI, and its problematic stability in ambient conditions poses concerns for its potential environmental impact. These concerns are motivating the search for novel non-toxic halide perovskites with similar optoelectronic properties to MAPI. In this work we will present the computational search for the homovalent and the heterovalent replacement of Pb in lead-halide perovskites. This search has lead to the computational discovery and experimental synthesis of two stable lead-free halide double perovskites based on Bi and Ag: Cs2BiAgCl6 and Cs2BiAgBr6. These new compounds are highly stable, they are semiconducting and absorb light in the visible range. In this talk we will present the electronic and optical properties of Cs2BiAgCl6 and Cs2BiAgBr6 calculated within DFT and GW and discuss the stability and formability of the entire Cs2BB'X6 family of semiconductors (B = Bi, Sb, B = Cu, Ag, Au, X = Cl, Br, I).

[1]This work was supported by the and the Leverhulme Trust (RL-2012-001).

Marina Filip
University of Oxford, Department of Materials

Date submitted: 10 Nov 2016 Electronic form version 1.4