Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Designing lead-free and stable perovskite materials for photovoltaic applications. YIYANG SUN, SHENGBAI ZHANG, Department of Physics, Rensselaer Polytechnic Institute — A critical barrier for large-scale deployment of the current perovskite solar materials is the use of Pb to achieve high power conversion efficiency. While this appears to be a technical issue, there are more fundamental reasons behind. The current research has mainly focused on the replacement of Pb by other elements, in particular, Sn. However, in halide perovskites (i.e., I-II-VII_3 composition), Sn is in its less stable 2+ state. The formation of more stable 4+ centers in the Sn(II)-based materials under ambient conditions makes the device efficiency very low. Worse, there might be no other elements across the Periodic Table that can replace Pb while maintaining the desirable properties, such as band gap. Out-of-the-box ideas are therefore called for to stimulate the research in this field. In this talk, two approaches are proposed based on state-of-the-art first-principles calculations. Through a screening of chalcogenide perovskite materials, $CaTiS_3$, $BaZrS_3$, $CaZrSe_3$, and $CaHfSe_3$ have been predicted to have suitable band gaps for making solar cells. Among these materials, $BaZrS_3$ have been synthesized experimentally. Another proposed approach is to introduce dual anions (i.e., splitting the anion sites) that allow the composition to satisfy charge neutrality, while replacing Pb by more environmentally benign elements. One of the candidate materials is $CH_3NH_3BiSI_2$, which is predicted to have band gap around 1.4 eV and high optical absorption.

Yiyang Sun
Department of Physics, Rensselaer Polytechnic Institute

Date submitted: 30 Nov 2015 Electronic form version 1.4