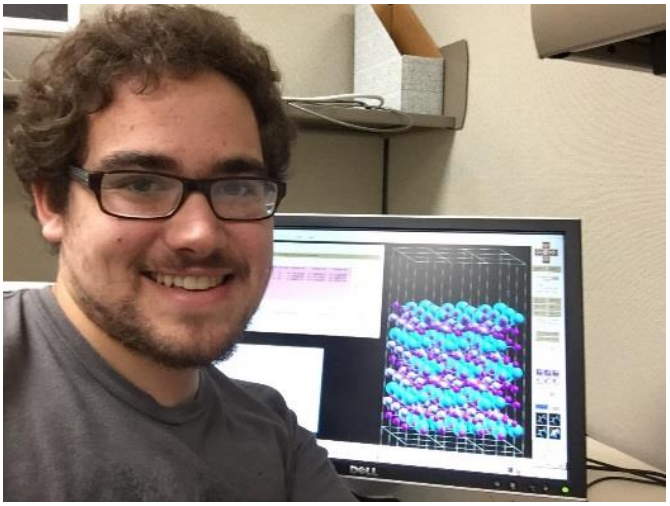

Thermodynamic Stability of CsPbI3 Surfaces
Mauricio Tassano (EAS 2017)
Advisor: Andrew Rappe

This summer I was a part of Dr. Andrew M. Rappe's theoretical research lab, where I investigated a class of materials that have intrigued scientists because of their outstanding performance in solar cells.

Halide perovskites have recently attracted a lot of scientific interest for their application in photovoltaics because of their high power conversion efficiencies. $CsPbI_3$ is one such inorganic material that is being investigated due to its similar performances with the most efficient perovskite found yet: $CH_3NH_3PbI_3$. It has been shown that $CsPbI_3$ takes two main configurations: *Pbnm* (active phase), in which the I_6 octahedron in the conventional unit cell shares a single halide atom with adjacent octahedrons, and *Pnma* (inactive phase), where two halide atoms are shared with adjacent octahedrons. For photovoltaic application, only the *Pbnm* phase can convert solar energy into useful energy. However, under ambient conditions bulk $CsPbI_3$ only forms the *Pnma* phase, which is non-functional for photovoltaic application. Thus the problem is being able to functionalize a *Pbnm* crystal configuration without having to assume very high temperatures or pressures. To spark our investigation, we found that recent experimental data seems to imply that the *Pnma* and *Pbnm* phase may coexist with one another near the surface. To investigate this we used thermodynamic principles and density-functional theory to create a $CsPbI_3$ phase diagram for a select number of systems, and thus determined which surfaces are energetically favorable at different environmental conditions. Our results in fact did confirm that within the bulk stability region of *Pnma* $CsPbI_3$, *Pbnm*-like surfaces are almost always energetically favorable. This is a fantastic result! To move this project forward we now hope to investigate the electronic structure and topology of our material in order to take another step towards materializing a functional $CsPbI_3$ perovskite solar cell under ambient conditions.

This research experience has taught me a lot about the current challenges facing the photovoltaic community over the realistic applicability of perovskite solar cells. Not only are there several scientific problems concerning stability, power conversion, and life-spans, but also there are some economic and environmental issues that need to be addressed. As a chemical engineering major, I

have realized throughout my studies at Penn the importance of energy in our society, and how often we take it for granted in this country especially. My time in the Rappe lab has taught me that there are so many different materials and interesting physics that are yet to be investigated, and that could help the world move away from burning fossil fuels and gravitate us towards becoming a clean energy society. I am going to continue my research this coming school year, and I hope to contribute as best I can towards smart climate action.

Thank you to CURF for rewarding me with a Penn Undergraduate Climate Action Grant so that I could pursue this research project, which I believe is vital to the maintenance and conservation of our society. Thank you so much!