Materials Science & Engineering Seminar Series

Carnegie Mellon University
Materials Science & Engineering

presents

Discovering Perovskites

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ABSTRACT:

In this talk I will illustrate how quantum-mechanical modeling of materials at the atomic scale plays an important role in solar energy research, and how it can be used to design and realize entirely new materials. After an introduction to solar photovoltaics, I will discuss the emergence of perovskite solar cells during the past few years, and explain why this family of materials has attracted so much interest in the scientific community. One of the outstanding challenges in perovskite research is to find new lead-free materials with optoelectronic properties comparable to lead-based halide perovskites. In this context I will discuss several approaches to the computational design of potential new perovskites and double perovskites, including concepts like cation substitution, band structure engineering, and combinatorial screening based on geometric descriptors. I will demonstrate that, when integrated with experimental synthesis and characterization, these approaches can deliver new materials with high potential for applications in solar energy harvesting and in energy-efficient lighting technology [1-3]. Furthermore I will show that we currently know only a small subset of all possible perovskites [4], and much more work is still needed to discover new materials of this family and to explore their uses in renewable energy technology.

[1] G. Volonakis, M. R. Filip, A. A. Haghighirad, N. Sakai, B. Wenger, H. J. Snaith, and F. Giustino, J. Phys. Chem. Lett. 7, 1254 (2016).

[2] G. Volonakis, A. A. Haghighirad, R. L. Milot, W. H. Sio, M. R. Filip, B. Wenger, M. B. Johnston, L. M. Herz, H. J. Snaith, and F. Giustino, J. Phys. Chem. Lett. 8, 772 (2017).

[3] G. Volonakis, N. Sakai, H. J. Snaith, and F. Giustino, J. Phys. Chem. Lett. 10, 1722 (2019).

[4] M. R. Filip and F. Giustino, Proc. Natl. Acad. Sci. 115, 5397 (2018).

BIOGRAPHY :

Feliciano Giustino received a M.Sc. degree summa cum laude in Nuclear Engineering form Politecnico di Torino, Italy, in 2001, and a PhD in Physics from the Swiss Federal Institute of Technology in Lausanne (EPFL), Switzerland, in 2005. During 2000-2001 he was a research fellow in the Experimental Physics Division of the European Laboratory for Particle Physics (CERN) in Geneva, Switzerland. During 2005-2008 he performed postdoctoral work at the University of California, Berkeley, and at the Lawrence Livermore National Laboratory. In 2008 he became University Lecturer in Materials Modelling at the University of Oxford, in the Materials Department, a position equivalent to Assistant Professor in the U.S., as well as Governing Body Fellow of Wolfson College, Oxford. In 2013 he was promoted to Associate Professor,and in 2014 to Full Professor of Materials at Oxford. In 2017 he was elected the Mary Shepard B. Upson Visiting Professor in Engineering at Cornell University, Ithaca, and spent a sabbatical leave in the Department of Materials Science and Engineering at Cornell in 2017-2018. In 2019 he was elected to the W. A. "Tex" Moncrief, Jr. Chair in Quantum Materials Engineering and Professor of Physics at the University of Texas at Austin. He is currently affiliated with the Oden Institute for Computational Engineering
and Sciences and the Department of Physics at UT Austin.

Feliciano Giustino specializes in electronic structure theory, high-performance computing, and the atomic-scale design of advanced functional materials. He is author of 120+ research papers and one book entitled "Materials Modelling using Density Functional Theory". He initiated the open-source software project EPW, which is now a core module of the Quantum ESPRESSO materials simulation suite and is regularly used by many research groups worldwide. He is the recipient of a European Research Council grant (2009) and of a Leverhulme Research Leadership Award (2012). He is primarily known for his work on electronic structure methods, and in particular for enabling accurate and efficient atomic-scale calculations of electron-phonon interactions and materials properties at finite temperature. More recently his work on materials design led to
the computational discovery and experimental realization of four new perovskites, to the filing and licensing of multiple patent applications, and to consulting roles in industry.

Friday, November 22, 2019
11:30AM - Doherty Hall 2210