Computation-Aided Materials Theory and Device Design for Photovoltaics and Electronics

Abstract: To meet surging demands for sustainable energy and environment, one critical factor lies in the advanced materials and devices for more efficient and eco-friendly energy production, conversion, and storage. Recent advances in quantum simulations of materials and high-performance computing have led to rapid development in computation-aided materials and device design. In this talk, I will highlight two examples of device design based on extraordinary properties of two-dimensional materials: (1) broad-spectrum solar energy funnel enabled by inhomogeneously strained two-dimensional ultrastrength materials, and (2) topological field effect transistor enabled by field dependent topological phases in a new class of quantum spin Hall insulators recently discovered in the two-dimensional transition metal dichalcogenides. I will also present two examples of methodology development towards accurate and efficient first-principles calculations, which will expedite high-throughput materials discovery and design for energy and device applications.

Bio of Dr. Qian: Dr. Xiaofeng Qian joined the Department of Materials Science and Engineering at Texas A&M University as an assistant professor in January 2015. He got his bachelor’s degree in Engineering Physics from Tsinghua University in China in 2001, and received his Ph.D. degree in Nuclear Science and Engineering from Massachusetts Institute of Technology in 2008. During his Ph.D. and first postdoctoral period, he worked with Prof. Sidney Yip and Prof. Nicola Marzari on the development of several first-principles methodologies for accurate and efficient predictions of electronic structures. From 2011 to 2014, he worked with Prof. Ju Li on two-dimensional materials and device design, including strain-engineered solar energy funnel and two-dimensional topological field effect transistor. Currently, his research focuses on two areas. One is the computation-aided materials discovery and design for energy applications and novel devices, and the other is the theoretical development for high-throughput prediction of physical and chemical properties of materials.

Contact yyao4 [at] uh [dot] edu (Prof. Yan Yao) if you would like to arrange for a time to meet with Dr. Qian.