CHEMISTRY & BIOCHEMISTRY COLLOQUIUM: From Many to Few Electrons: An Overview of Electronic Structure Theory and Applications at Cal State East Bay

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Date:
12/10/2021

Time:
1:30 PM-2:50 PM

Link:
COB1 267

About the Speaker:

Patrick Huang's primary focus is on undergraduate education and mentorship. As an Associate Professor at Cal State East Bay, he teaches courses ranging from introductory chemistry for non-science majors, to Masters-level courses in computational chemistry. His research program with undergraduate students examines both fundamental and environmental aspects of actinide chemistry. Prior to Cal State East Bay, he was a Staff Scientist in the Quantum Simulations Group at Lawrence Livermore National Laboratory where he studied the structure and dynamics of solid/aqueous interfaces.

Abstract:

Chemical bonding in actinide compounds may be viewed as an extreme limit where relativistic effects are significant and correlation effects are complex. In this talk, I will give an introduction to actinide bonding, with an emphasis on first-principles theoretical methods for analyzing bond character. These methods are applied to examine the bonding in some recently synthesized U(IV) and Th(IV) coordination complexes with remarkably short metal-phosphorous and metal-arsenic bonds. The insights from the computations, in conjunction with X-ray and nuclear magnetic resonance data, suggest that these bonds possess significant multiple-bond character. Finally, I will describe our progress towards the development of grid-based techniques for the solution of quantum few-body problems that involve both electronic and nuclear degrees for freedom.

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