Modeling many-body interactions for materials design: From quantum dots to clathrates

Seminar

Friday, November 15, 2024

2:00 – 3:00 p.m.

Beaupre Center, Room 105

Accurately describing many-body interactions remains a challenge in theoretical and computational chemistry, yet it is key to understanding and optimizing the performance of materials relevant to applications, such as quantum information and energy conversion. Here, I will describe my work to model many-body interactions in two distinct materials. First, I will discuss quantum dots (QDs), which are semiconducting nanocrystals with highly tunable optoelectronic properties that depend sensitively on interactions between electronic excitations and phonons (i.e., lattice vibrations). We develop and validate an approach to describe exciton-phonon coupling with atomistic detail in QDs of experimental relevance with 100s of atoms. We simulate energy dissipation and find that it occurs on ultrafast timescales, in agreement with experimental results but contrary to longstanding theoretical expectations. Furthermore, we identify QD handles for tuning these timescales to reduce thermal losses and increase quantum yield. Next, I will focus on clathrate solids, which are cage-like chemical structures that are promising for thermoelectric applications due to their strong phonon-phonon interactions (i.e., anharmonicity). We develop and apply vibrational dynamical mean-field theory (VDMFT), a method based on quantum embedding, to simulate anharmonicity and thermal transport in clathrates. We show that VDMFT is both efficient and accurate, describing multi-phonon scattering processes that underlie clathrates' unique vibrational dynamics but that are neglected in common perturbation theory approaches. With the predictive power enabled by the tools described in this talk, we are better positioned to unlock transferrable insight for enhanced materials design.

Dipti Jasrasaria
Department of Chemistry
Columbia University

THE UNIVERSITY OF RHODE ISLAND

Department of Chemistry

Fall 2024 Seminar Series

Host: **Dugan Hayes**
Associate Professor
dugan@uri.edu
401-874-5516 (office)
617-785-4633 (mobile)