



## 25<sup>th</sup> Anniversary Luncheon

**Coordinator:** Lorena Tribe (lut1@psu.edu)

**Talk Title:** "Coarse-Graining Solvents using Stochastic Hard Collisions"

**Presenter:** Rigoberto Hernandez, Ph.D., Johns Hopkins University



**Abstract:** The structure of coarse-grained particles is known to be recoverable from models with bounded potentials such as the penetrable sphere model or more complicated soft-interaction models. We have developed a stochastic hard collision model that allows one to effectively capture the structure arising from a corresponding soft-particle model while allowing for the computational efficiency arising from hard-particle models [J. Chem. Phys. 138, 244901 (2013)]. We will report the extent to which this model provides correct dynamics at coarse-grained time-scales. The efficiency of the SHC model also provides an alternative to fine-grained solvent models for the characterization of the motion or reactions of finer-grained solutes.

**Time:** Tuesday, June 6 from 12 pm - 1:30 pm

**Room:** Tower 1

**Notes:** This room fits 40 banquet style. There are other MoleCVUE talks and activities that are part of the technical session on Sunday afternoon, Tuesday morning and Tuesday afternoon.