



Contribution ID: 130 Contribution code: Board 5

Type: Poster Presentation

Explorations of the Molecules-to-Materials Continuum

Monday, May 20, 2024 7:10 PM (20 minutes)

A continuum in the chemical space linking molecules and materials encompasses promising physical and chemical properties that both extremes do not and cannot display. As we consider transitioning from well-defined structures and compositions toward materials, their surfaces, and grain boundaries through nanoparticles, new chemical reactivity, catalytic properties, and unique chemical functions may hide in plain sight. We have been exploring various continuums established for aluminosilicates [1], iron-sulfur nanoparticles [2], and carbon materials [3], as representative examples for hard, tender, and soft materials, respectively. Our ambitious effort is the bridging of acid/base chemistry of exfoliated clays nanoparticles and Fe-S clusters with rich redox chemistry toward generating organic compounds and materials. Computational molecular cluster models, as maquettes of reactive sites of interest are being employed for studying physisorption on CH_4 and H_2 on carbon surfaces, reactivity of H_2 , H_2S , and other small organic molecules with on hybrid Fe-S-clay nanoparticles. The computational work is driving the atomic-level interpretation of spectroscopic features (FTIR, EPR, XANES/EXAFS) and analytical measurements (DTG/DSC-MS). X-ray synchrotron spectroscopy offers the connection between theoretical modeling and experimental work due to mining electronic and geometric structural information for the reactive sites, as a key technique in validating the accuracy of theory and the adequacy of the computational maquettes.

Primary author: SZILAGYI, Robert (The University of British Columbia - Okanagan)

Presenter: SZILAGYI, Robert (The University of British Columbia - Okanagan)

Session Classification: Poster Session

Track Classification: Poster Presentations