Mesoscale Priority Research Direction

Shuffling Materials Chemistry: Controlling emergent phenomena in layered materials

Opportunity

Many materials system are well known and well behaved on the molecular or bulk levels. To explore and develop new materials to meet growing challenges in materials science for molecularly engineered systems with unprecedented optical, structural, reactive, or catalytic properties, one should explore novel layered materials whereby new properties are developed through manipulating and controlling inter- and intra-layer chemistries.

Meso Challenge

The great advances that have emerged in mesoscale materials have been inspired by biological systems such as nacre in abalone, small single crystals of aragonite layered with biopolymers. Lacking in the meso area of science is the ability to replicate inspiration such as this at the molecular and submicron level and have the tools to characterize, understand, and model the new systems and their resulting properties.

Approach

To address this challenge, new paradigms can be used that consider layered materials as starting points and further refining via directed synthetic means coupled with computational methods in a predicative manner. Pairing chemistry, solid-state physics and computational teams is key to understanding the complexity of the mesoscale problem.

Materials that are molecularly ordered, have long-range structure, yet are at some level disordered pose one of the most difficult systems to study. Multi-pronged approaches that utilize National User Facilities (LANL, PNNL, ORNL) give researchers the highest chance for teaming and success.

Impact

Two things will emerge from achievement in this emerging scientific field. (1) A toolbox with building blocks and assembly methods to create robust materials ordered and disordered at the mesoscale. (2) Characterization methods to correlate ordering and performance at the molecular, micron, and long-range scale.

References: **Design principles for oxygen-reduction activity on perovskite oxide catalysts for fuel cells and metal–air batteries** J. Suntivich *et al.*, Nature Chemistry 3 (2011) 546–550. **Prying Apart Ruddlesden–Popper Phases: Exfoliation into Sheets and Nanotubes for Assembly of Perovskite Thin Films,** R.E. Schaak *et al.,* Chem Mater 12 (2000) 3427–3434. **Stable single-unit-cell nanosheets of zeolite MFI as active and long-lived catalysts,** M. Choi et al., Nature 461 (2009) 246-249.**Triblock Copolymer Syntheses of Mesoporous Silica with Periodic 50 to 300 Angstrom Pores,** Zhao et al., Science 279 (1998) 548-552.

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