CALIFORNIA STATE UNIVERSITY FULLERTON
NATURAL SCIENCES AND MATHEMATICS

CCAM
Center for Computational and Applied Mathematics

CCAM presents:

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Seminar Topic

Modeling the properties of hybrid organic-inorganic materials

The behavior of hybrid materials is relatively unexplored compared to that of purely organic or inorganic materials and can be remarkably different. A striking example of this is the porous metal-organic framework UiO-66, which has a concentration of missing-linker defects that can exceed 10% depending on the synthesis conditions. We use a combination of Monte Carlo simulations, density functional theory (DFT) and force field calculations to study the structure and interactions of those defects, and their influence on the electronic structure of the material. [1]

Another difference between inorganic and hybrid materials are in their mechanical properties. Hybrid materials are mechanically soft, which might have consequences for properties such as magnetic or ferroelectric ordering. Using DFT we investigate the mechanical and temperature-dependent behavior of the ferroelectric formate perovskite $[NH_2NH_3][Zn(CHO_2)_3]$, showing how the thermal movement affects the ferroelectric ordering.

[1] J. K. Bristow, K. L. Svane, D. Tiana, J. M. Skelton, J. D. Gale and A. Walsh, J. Phys. Chem C **120**, 9276 (2016)

Friday, September 16, 2016
Location: MH – 552
Time: 11:00 a.m.
Refreshments will be served
For questions email: ccam@fullerton.edu