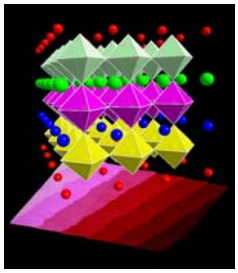
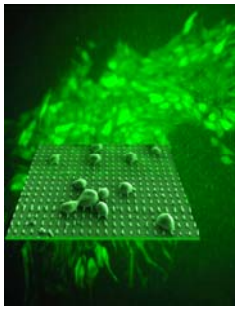
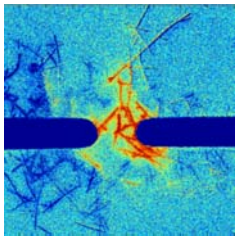
CNMS DISCOVERY SEMINAR SERIES







Friday, May 14, 2010
11:00 am
Iran Thomas Auditorium, 8600

New Materials for Solar Photovoltaic Applications

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Abstract:
Solar energy is a promising long-term solution for future energy requirements; however, current solar energy conversion devices are plagued by low efficiency. The use of ferroelectric ABO_3 perovskite oxides is one approach for boosting conversion efficiency and reducing cost. Ferroelectric oxides possess spontaneous polarization and have been shown to produce a bulk photovoltaic effect in which charged carriers (e- and h+) separate to prevent recombination. Once separated, the high-energy electrons are available for electrical work or for the catalytic splitting of water into hydrogen and oxygen. Currently, most solid oxide ferroelectrics have a band gap of at least 3 eV, absorbing primarily in the ultra-violet (UV) region. Since UV light comprises only 8% of the solar spectrum, new materials with a decreased band gap and large polarization would be highly desirable.

In this talk, we will report the results of computational materials design to increase the light absorption and carrier separation in ABO_3 oxides. To reduce the band gap and increase light absorption, we substitute the B site of Pb-based perovskites with elements whose bonds with oxygen are less ionic and more covalent. We also devise substitutions that keep the material polar, enhancing charge separation. We particularly focus on substitution of the B-site of $PbTiO_3$ with group 10 metals Ni, Pd and Pt, stabilized by an accompanying O vacancy. The resulting materials are new semiconducting ferroelectric oxides that are promising candidates for solar light harvesting.

Host: Art Baddorf, baddorfap@ornl.gov, 865.574.5241

Center for Nanophase Materials Sciences