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Research Summary: The research focus is on the use of nanoscale oxides as energy materials. Select problems of interest include:

- Mechanisms of early stages of oxidation and nanoscale oxide growth on binary and ternary alloy metal substrates
- Tuning oxide functional properties by athermally controlling the composition, stoichiometry and density of multi-component oxides
- Ion dynamics at water-oxide interface for catalytic and energy applications
- Structure-property relationships in low dimensional systems such as transition metal alloy nanomaterials
- Nanoscale ion transport through oxide materials and its relevance to corrosion phenomena in electrochemical environments

The main focus is on the development of computational models and simulation techniques to address the above problems. Particular emphasis is on the development and utilization of atomistic simulation techniques such as Molecular dynamics & Monte-Carlo. Other techniques of interest include electronic structure calculations based on density functional theory and continuum level approaches such as finite element method.

Selected Recent Publications:

1. Sankaranarayanan, Subramanian K. R. S., Efthimios Kaxiras and Shriram Ramanathan. ***Atomistic simulations of field enhanced oxidation of Al(100) beyond the Mott potential.*** Physical Review Letters, 102, 095504 (2009).
2. Sankaranarayanan, Subramanian K. R. S. and Shriram Ramanathan. ***On low temperature oxidation and ultra-thin oxide growth on Zirconium surfaces in presence of atomic oxygen: A modeling study.*** Journal of Physical Chemistry C, 112, 17877 (2008).
3. Sankaranarayanan, Subramanian K. R. S. and Shriram Ramanathan. ***Molecular dynamics simulation study of nanoscale passive oxide growth on Ni-Al alloy surfaces at low temperatures.*** Physical Review B, 78 085420/1-17 (2008).
4. Sankaranarayanan, Subramanian K. R. S.; Bhethanabotla, Venkat R.; Joseph, Babu. ***Molecular dynamics simulation study of temperature and strain rate effects on the elastic properties of bimetallic Pd-Pt nanowires.*** Physical Review B (2007) 76, 134117/1-13.
5. Sankaranarayanan, Subramanian K. R. S.; Bhethanabotla, Venkat R.; Joseph, Babu. ***Molecular dynamics simulation study of the melting and structural evolution of bimetallic Pd-Pt nanowires.*** Physical Review B (2006), 74(15), 155441/1-155441/12.
6. Sankaranarayanan, Subramanian K. R. S.; Bhethanabotla, Venkat R.; Joseph, Babu. ***Molecular dynamics simulation study of the melting of Pd-Pt nanoclusters.*** Physical Review B (2005), 71(19), 195415/1-195415/15.