Physics & Astrophysics Colloquium

Multiscale Material Modeling
Insight from Bulk to the Surface

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4:00 PM Friday, September 16, 2022
Room 211, Witmer Hall

Abstract:

Fundamental advances in computational methods are key in the discovery, understanding and optimization of materials. Quantum mechanical approach alongside molecular and thermodynamic methods has been successfully employed in the search for new materials, understand/optimize the properties of existing materials for different applications. We have employed this strategy for energy, oil/gas and medical physics applications. Specifically, our investigation of solid oxide fuel cell involved a detailed understanding of structural, electronic and defect formation characteristics, for a rational design of cathode materials. We demonstrated that anisotropy effects often neglected at high operating temperature becomes relevant when temperature is lowered. We investigated the role of defects on the ionic transport in the different classes of materials employed for this application. Same approach was employed to study materials used as scintillators for medical application. Here we investigated degradation often encountered in scintillators while in operation due to defects induced in the process. Overcoming this menace require an extensive understanding of the defect process. Knowledge of the defect formation process is also important in the design of resilient scintillators. Furthermore, using a combination of first-principles, molecular dynamics and Darwin evolutionary algorithm, we predicted crystal structures of 2D hybrid organic-inorganic perovskites for solar and memristor application. While all of the systems studied above were bulk systems, understanding and application of these research tools was helpful in the investigation involving surfaces of systems. Specifically, in the design of efficient systems that inhibit corrosion on metallic surfaces. we studied the corrosive disintegration of metals and their alloys into fine particles and organometallics occurring in carbon saturated environment at catalytic operating temperatures. This menace leads to serious economic implications on several industrial processes especially in the oil and gas sector. Our findings show that the orientation and nature of the syngas play a significant role in determining the rate limiting step and controlling surface chemistry of gaseous reactions on metal surfaces.

Refreshments at 3:30 PM in Witmer Hall, Room 215

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