**Motivation**

- Due to the unusual properties and non-linearity from partially filled d orbitals, perovskite structure materials (e.g., strontium titanate (STO)) and their doped systems (e.g., La-doped STO) attract researchers’ great attention and possess a wide range of applications, such as a dielectric material in capacitor, an oxygen ion conductor as in sensor and solid oxide fuel cell (SOFC), as a piezoelectric material in actuator, as a substrate material in capacitor, as an oxygen ion conductor as in sensor and SOFC.

- Theoretical modeling is a powerful tool to explore the electronic, optical, and thermodynamic properties of these solids at high temperature. Employing with atomistic-level simulation methods (first-principles DFT, and thermodynamic properties of these solids at high temperature.

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**Applications**

- Atomistic Modeling of Functional Materials for Sensor and SOFC

**Perovskite Materials**

- Ab initio thermokinetic modeling of cation transport for SOFC cathode degradation
  - New dominant A-site cation migration mechanism identified: \( V_{\text{HoP}} - V_{\text{O}}^{\text{p}} \) = 1.6 eV
  - Comparable A-site and B-site cation migration barriers involving \( V_{\text{HoP}}^{\text{p}} - V_{\text{O}}^{\text{p}} \) = 1.6 eV
  - Predict \( D_{\text{O}}^{\text{p}} \) and \( D_{\text{Mn}}^{\text{p}} \) vs. \( T, P(O_{2}) \), Sr doping

**Temperature Effects: TiO₂**

- Optical-based sensing platforms, especially the Au-nanoparticle incorporated plasmonic oxides, such as Au-TiO₂, have shown the potential for robust and reliable optical gas sensing properties at high temperature. We performed DFT-based simulations to get a fundamental understanding of the temperature effect on the electronic and optical properties of rutile and anatase TiO₂.

**Li diffusion pathways in γ-LiAlO₂**

- The study of H and Li diffusivity in Li containing ceramics has been a subject of interest in Li-ion battery, SOFCs, and tritium science and technology. Using first-principles density function theory (DFT), here we study the mechanisms associated with atomic H and Li diffusion kinetics in γ-LiAlO₂. In particular, we show diffusion pathways for interstitial and substitutional H defects, hydroxide (OH) vacancy defects, interaction of H with O-vacancies and lattice Li atom in ceramic γ-LiAlO₂.

**Electronic structure**

- The temperature effect on band gap is contributed by electron-phonon interaction: the thermal expansion.

**Potential applications** for high-T gas sensor and SOFC.