Atomistic Modeling of Functional Materials for Sensor and SOFC Applications

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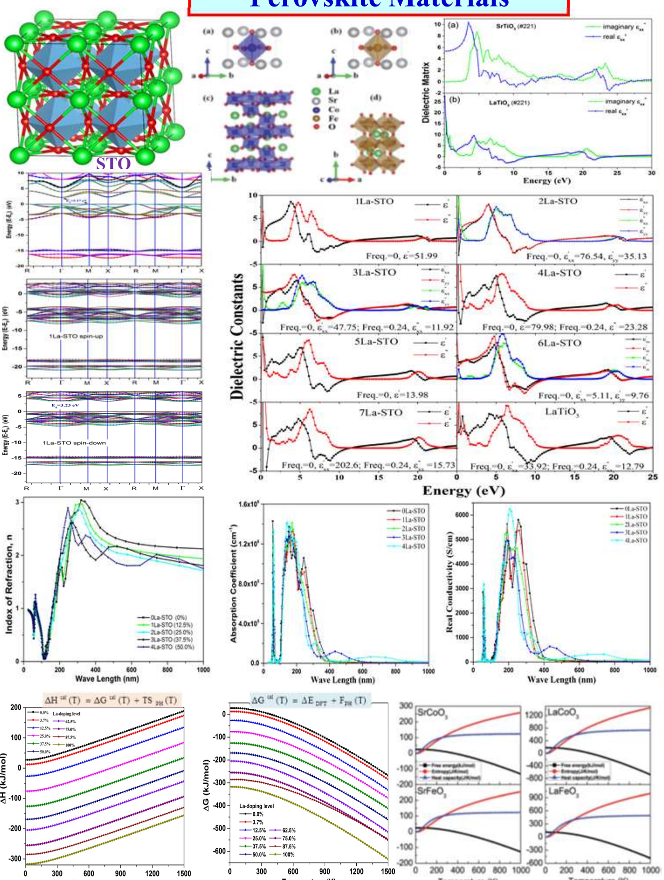
Motivation

- 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) attracts researchers' great attention and possesses a wide range of applications, such as a dielectric material in capacitor, as an oxygen ion conductor as in sensor and solid oxide fuel cell (SOFC), as a piezoelectric material in actuator, as a substrate for high Tc superconductor, as a thermoelectric material with low thermal conductivity and high electrical conductivity due to the enhanced electronic transport, and *etc*.
- Theoretical modeling is an powerful tool to explore the electronic, optical, and thermodynamic properties of these solids at high temperature. Employing with atomistic-level simulation methods (fist-principles DFT, MD, lattice dynamics, *etc*.), we have been investigating several materials with potential applications for high-T gas sensor and SOFC.

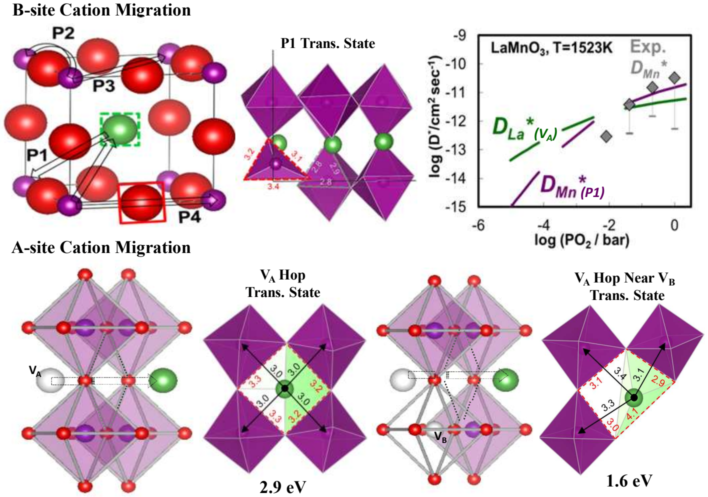
Perovskite Materials



Ab Initio Modeling of Cation Diffusion in $La_{1-x}Sr_xMnO_{3\pm\delta}$ for SOFC:

Develop quantitative models to assess cation diffusivities in bulk LSM vs. T, pO_2

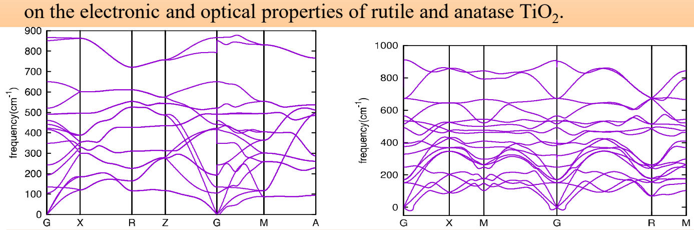
DFT and Bulk Defect Thermokinetic Modeling



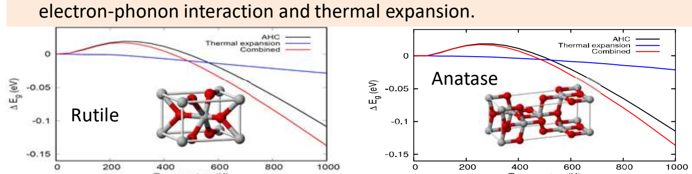
- *Ab initio* thermokinetic modeling of cation transport for SOFC cathode degradation
  - New dominant A-site cation migration mechanism identified- $(V_A''' - V_B''')$:~1.6 eV
  - Comparable A-site and B-site cation migration barriers involving $(V_A''' - V_B''')$ cluster carriers
- Predict D_{La}^* and D_{Mn}^* vs. T, $P(O_2)$, Sr doping

Temperature Effects: TiO_2

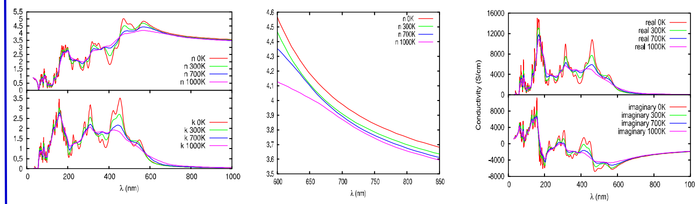
- Optical-based sensing platforms, especially the Au-nanoparticle incorporated plasmonic oxides, such as Au/TiO_2, have shown the potential for robust and reliable optical gas sensing properties at high temperature. We performed DFT-based simulations to get a fundamental understanding of the temperature effect on the electronic and optical properties of rutile and anatase TiO_2.



- **Electronic structure**: The temperature effect on band gap is contributed by electron-phonon interaction and thermal expansion.

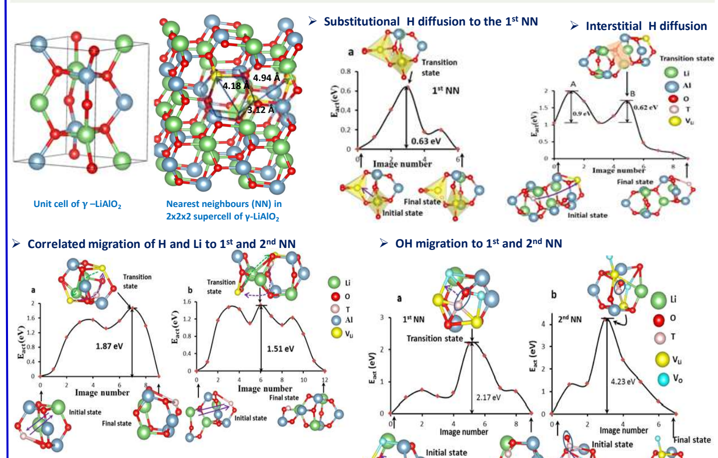


- **Optical property**: The refraction index (n), extinction coefficient (k), and the optical conductivity curves are smoothed by temperature.



Li diffusion pathways in r-$LiAlO_2$

- 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 r-$LiAlO_2$. 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-$LiAlO_2$.



Publications

(1) Y. Duan, C. D. Stinespring, B. Chorpening, "*Electronic structures, bonding configurations, and band-gap opening properties of graphene binding with low-concentration fluorine*", **ChemistryOPEN**, **4**(2015)642-650

(2) Y.-L. Lee, Y. Duan, D. Morgan, D. Sorescu, H. A. Abernathy, and G. Hackett, "*Density Functional Theory Modeling of A-site Cation Diffusion in Bulk* $LaMnO_{3\pm\delta}$ *for Solid Oxide Fuel Cell Cathodes*", **ECS Transactions, 78**(2017) 2797-2806

(3) Y. Duan, P. Ohodnicki, B. Chorpening, H. Abernathy, G. Hackett, "*Theoretical Investigation of the Electronic Structural, Optical and Thermodynamic Properties of* $La_xSr_{1-x}TiO_3$ *(x=0, 0.125, 0.25)*", **ECS Transactions**, **78**(2017) 2865-2876,

(4) T. Jia, Zhi Zeng, H. Q. Lin, Y. Duan, P. Ohodnicki, "*First-principles study on the electronic, optical and thermodynamic properties of* ABO_3 *(A = La, Sr, B = Fe, Co) perovskites*", **RSC Advances, 7**(2017)38798-804.

(5) Y. Duan, P. Ohodnicki, B. Chorpening, G. Hackett, "*Electronic structural, optical and phonon lattice dynamical properties of pure- and La-doped* $SrTiO_3$*: an ab initio thermodynamics study*", **J. Solid State Chem. 256**(2017)239-251

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(7) X.-L. Zhang, M.-M. Han, Z. Zeng, Y. Duan, "*The role of Sb in solar cell material* Cu_2ZnSnS_4", **J. Mater. Chem. A 5**(2017)6606-66012

(8) H. P. Paudel, Y.-L. Lee, D. L. Senor, Y. Duan, "*Tritium Diffusion Pathways in γ-*$LiAlO_2$ *Pellets Used in TPBAR: a first-principles density functional theory investigation*", **J. Phys. Chem. C** (2018) submitted.

(9) Y.-N. Wu, W. A. Saidi, P. Ohodnicki, B. Chorpening, Y. Duan, "*Temperature effect on electronic structure and optical properties of rutile* TiO_2", **Physical Review B** (2018) to be submitted.

(10) Y. Duan, B. Chorpening, C. D. Stinespring, "*A first-principle study of the optical properties of low-concentration fluorine doped graphene*", (2018) to be submitted.

(11) Y.-L, Lee, J. Holber, H. Paudel, D. C. Sorescu, D. Sensor, Y. Duan, "*Density Functional Theory Study of the Point Defect Properties for the γ-*$LiAlO_2$*,* Li_2ZrO_3*, and* Li_2TiO_3 *Materials*", (2018) to be submitted

(12) Y. Duan, Dan C. Sorescu, D. Senor, "*Electronic structural, optical, lattice thermodynamic, and thermo-conductive properties of γ-*$LiAlO_2$ *with* ^6Li *isotope substitutions for tritium production: A DFT approach*", (2018) to be submitted.

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