School Seminar (2015-28)

School of Materials Science & Engineering

"Explosive phase transitions revealed by quantum materials genome study in this-film oxides"

Prof. Lee, Jun Hee

(School of Energy & Chemical Engineering, UNIST)

2015. 09. 18. (Fri.) 13:00

APRI 1F, Auditorium Hall

Explosive phase transitions revealed by quantum materials genome study in this-film oxides

Jun Hee Lee (School of Energy & Chemical Engineering, UNIST)

In an organism, the unique structure and subsequent function of a protein are determined singly by the gene sequence. Genome research such as the *Human Genome Project*, aided by advanced computation technology, have begun to unlock the complexity surrounding gene sequence and its role in determining biological function, bringing about significant advances in biotechnology and medicine. In this spirit, we initiate **quantum materials genome** research, which can combine many condensed-matter issues with computation. In the condensed matters, a well-defined order parameter such as spin, charge, symmetry, and lattice can be seen as material genes. Unlocking their coupling/combination and its manifestation in the hierarchical materials imply endless possibilities for material engineering and design, and hold the key for creating new phases out of old materials. By applying quantum materials genome method, first, I will talk about how to induce drastic phase transitions by altering the largest magnetic interaction, which is superexchage in oxides, via its coupling to lattice distortions such as ferroelectric [1,2,3] or Jahn-Teller [4]. Second, I will discuss how to switch on/off non-zero net magnetic moments by electric-field in oxide superlattices such as $BiFeO_3/LaFeO_3$ through combined study of density functional theory, spin models and neutron scattering technique. Third, by stacking conventional catalysts on high-*k* material, dynamic response is endowed to rapidly-changing charged-intermediate molecules and accelerate various photocatalytic reactions such as water-splitting [5,6]. Overall, I will highlight the importance of systematic genome study of various order-parameters to reveal hidden phases and maximize photo-catalytic capabilities in thin-film oxides.

[1] "*Epitaxial-Strain-Induced Multiferroicity in $SrMnO_3$ from First Principles"*, J. H. Lee and K. Rabe, **Physical Review Letters**, **104**, 207204 (2010).

[2] "*Coupled Magnetic-Ferroelectric Metal-Insulator Transition in Epitaxially Strained $SrCoO_3$ from first principles*", J. H. Lee and K. Rabe, **Physical Review Letters**, **107**, 067601 (2011).

[3] "Huge spin-driven polarizations in bulk BiFeO3 at room-temperature" J. H. Lee and R. Fishman, **Physical Review Letters** (in press) (2015).

[4] "*Strong coupling of Jahn-Teller distortion to oxygen-octahedron rotation and functional properties in epitaxially-strained orthorhombic $LaMnO_3$*", J. H. Lee *et al*., **Physical Review B**, **88**, 174426 (2013)

[5] "*Incorporation of Nonmetal Impurities at the Anatase TiO_2(001)-(1×4) Surface*", J. H. Lee and A. Selloni, **Physical Review Letters 110**, 016101 (2013).

[6] "*Dynamically-induced-dipoles enhance photocatalytic oxygen evolution on $TiO_2/SrTiO_3$ heterostructures*", J. H. Lee and A. Selloni, **Physical Review Letters**, **112**, 196102 (2014).

Jun Hee Lee

Curriculum Vitae

Ulsan National Institute of Science & Technology
School of Energy & Chemical Engineering
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■ EDUCATION

2003-2008 **Doctor of philosophy,** Theoretical Solid-State Physics
Computational Nano-Material Physics Laboratory
Department of Physics, Seoul National University, Seoul, Korea (Supervisor : Prof. Jaejun Yu)

Dissertation *First-principles effective Hamiltonian study of ferroelectric perovskite oxide superlattices.*

- Discovering best combinations of transition-metal oxide nanostructures for enhanced ferreoelectric performance with using localized-phonon-Wannier functions
- Understanding surface reconstruction and electronic structure of nano-sized diamond and designing porous but hard nano-size clusters.

2001-2003 **Master of Science,** Physics, Seoul National University, Korea (Supervisor : Prof. Jaejun Yu)

Thesis *Fullerene-like reconstructions of nano-diamond surfaces.*

1997-2001 **Bachelor of Science,** Physics, Seoul National University, Korea (Supervisor : Prof. Yung-Woo Park)

Thesis *Transport properties of conducting polymers.*

■ RESEARCH EXPERIENCE

2013~present **Post-doctoral Fellow,** Materials Science & Technology Division, Oak Ridge National Lab., USA

Mentor Dr. Randy Fishman

Research Modeling Coupled Spin-Lattice-Photon Dynamics in Transition-Metal Oxides

- Revealing magneto-electric couplings in organic-inorganic hybrid nanostructures by combining various models with quantum-mechanical calculations
- Computational nano-optics for light-matter interactions by reproducing time-resolved Raman- and optical-spectroscopy in oxide materials by using linear-response theory
- Understanding uni-directional light propagations and designing optical diode via light-spin-lattice interaction in transition-metal oxides

2011-2013

Mentor **Post-doctoral Fellow,** Department of Chemistry, Princeton University, USA

Research Professor Annabella Selloni

Computational Design of Molecular Reactions on Photoelectro-Catalystic Surfaces

- Design of improved oxygen-reduction and oxygen-kinetic processes on quantum-paraelectric transition-metal oxides for effective water splitting, CO_2 conversion, and fuel cells
- Catalysts@ferroelectric core-shell nano-structures for breaking covalent- and hydrogen-bonds of molecules and accelerating charge- and proton-transfer dynamics in catalytic reactions
- Control of surface doping characteristics (interstitial vs. substitution) and concentration to promote selective photo-catalytic reactions and increase photo-excited-carriers mobility

2008-2011

Mentor

Research **Post-doctoral Fellow**, Condensed Matter Theory Group, Rutgers University, New Jersey, USA.

Professor Karin M. Rabe

Initiating "***Quantum Materials Genome (QMG)"*** research for revolutionary crystal engineering

- Systematic understanding of hierarchical structure-property relationship digitalized by computation for quantum oxides, inspired by human genome research
- Designing Room-*T* ferroelectric-ferromagnetic transition-metal oxides through *QMG*
- Deigning ferromagnetism controllable by electric-field for energy-efficient memory

Sep.-Dec. 2010 **Visiting Scholar**, University of California, Santa Barbara, USA.

Collaborator Professor Nicola Spaldin

Research — Understanding complex oxides for HOMO-LUMO level engineering for functional nanomaterials

- Utilizing coupling between Jahn-Teller distortion and oxygen-octahedron rotation for the control of band-gap for improved photon absorption
- Strain-engineering of HOMO-LUMO level positions by controlling of Jahn-Teller distortion for allowing the molecules such as water to be both oxidized and reduced effectively

2006~2007 — **Research Intern**, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India.

Collaborator Research — Professor Umesh V. Waghmare

Effective Hamiltonian using localized phonon Wannier functions for the calculation of large-size ferroelectric nanostructures with *ab-initio* simulation

Computational Capabilities — Expertise in VASP, SIESTA, Quantum ESPRESSO, ABINIT, Open-MX (LCAO)
FERAM (MD simulation for bulk, thin-film, and nano-structure)