

Curriculum Vitae

Byung-Hyun Kim

Platform Technology Laboratory, Korea Institute of Energy Research, Republic of Korea
Tel: +82-42-860-3218, e-mail: bhkim@kier.re.kr

WORK EXPERIENCE

- **Senior Research Scientist** Jul. 2017 – present
Platform Technology Laboratory, Korea Institute of Energy Research
- **Postdoctoral Researcher** Feb. 2016 – Jun. 2017
Department of Chemistry–Ångström Laboratory, Uppsala University, Sweden
- **Senior Engineer** Mar. 2013 – Jan. 2016
CAE Team, Semiconductor R&D Center, Samsung Electronics Co., Ltd.
- **Research Assistant (Direct-General: Dr. Kwang-Ryeol Lee)** Feb. 2008 – Feb. 2013
Center for Computational Science, Korea Institute of Science & Technology

EDUCATION

- **Ph.D.**, February 2013 (Supervisor: Prof. Yong-Chae Chung & Dr. Kwang-Ryeol Lee)
Department of Materials Science & Engineering, Hanyang University, Seoul, Korea
Dissertation: Multiscale Simulation Study of Interfacial Properties on Low Dimensional Materials: CNTs and SiNWs
- **M.S.**, February 2009, Department of Materials Science & Engineering, Hanyang University
- **B.S.**, February 2007, Department of Ceramic Engineering, Hanyang University

EXPERTISE

- **Electronic structure calculations of energy materials, thermodynamics, surface/defect chemistry, catalysis**
- **Atomic-level Simulations:** density functional theory (DFT), density functional based tight binding (DFTB), kinetic Monte Carlo (kMC), non-equilibrium Green's function (NEGF), and classical and reactive molecular dynamics (MD)
- Atomic/device simulation packages: VASP, SIESTA, DFTB+, LAMMPS, Sentaurus tools (Synopsys)
- C, C++, Python, Shell script

PATENTS

- Multi Dimensional Virtual Experimental Apparatus and Method for Nano Device Design (Korea, USA, EU)
- Method of Fabricating Co-Cu Thin Film Multilayers of Optimized Deposition Condition by Molecular Dynamics Simulation (Korea)

SELECTED PUBLICATIONS

- Multiscale Modeling of Agglomerated Ceria Nanoparticles: Interface Stability and Oxygen Vacancy Formation [*Frontiers in Chemistry* 7:203 (2019)]
- Facile Synthesis of a High Performance NiPd@CMK-3 Nanocatalyst for Mild Suzuki-Miyaura Coupling Reactions [*ChemCatChem* 11, 991 (2019)]
- Indirect-to-Direct Band Gap Transition of Si Nanosheets: Effect of Biaxial Strain [*The Journal of Physical Chemistry C* 122, 15297 (2018)]
- Functionalization effect on Pt/carbon nanotube composite catalyst: A first-principles study [*Physical Chemistry Chemical Physics* 18, 22687 (2016)]
- Effects of Suboxide Layers on the Electronic Properties of Si(100)/SiO₂ Interfaces: Atomistic Multi-scale Approach [*Journal of Applied Physics* 113, 073705 (2013)]
- Stress Evolution during the Oxidation of Silicon Nanowires in the Sub-10 nm Diameter Regime [*Applied Physics Letters* 99, 143115 (2011)]
- Improved Binding between Copper and Carbon Nanotubes in a Composite using Oxygen-containing Functional Groups [*Carbon* 49, 811 (2011)]