<Professor Yong-Hoon Kim's Lab.>`

Atomic-Scale Devices Simulation Lab

■ **Contact information**

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■ **Current state of the Lab. (in 2025 Spring Semester)**

Postdoctoral Fellows: 2 PhD Students: 5 Master's Students: 2 Secretary: 1

■ **Research Areas**

1st-principles (atomic-scale) electronic structure, quantum transport, & technology computer-aided design (TCAD) simulations

1. Theory & Computation

- semiconductor physics & electronic structure theory behind the TCAD technology
- high-performance computing (HPC) and artificial intelligence (AI) / machine learning (ML) acceleration

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2. Functional Nano-Materials

- low-D vdW materials (graphene, TMDC, etc.)
- halide perovskites, oxides, etc.
- quantum dots, wires, & wells

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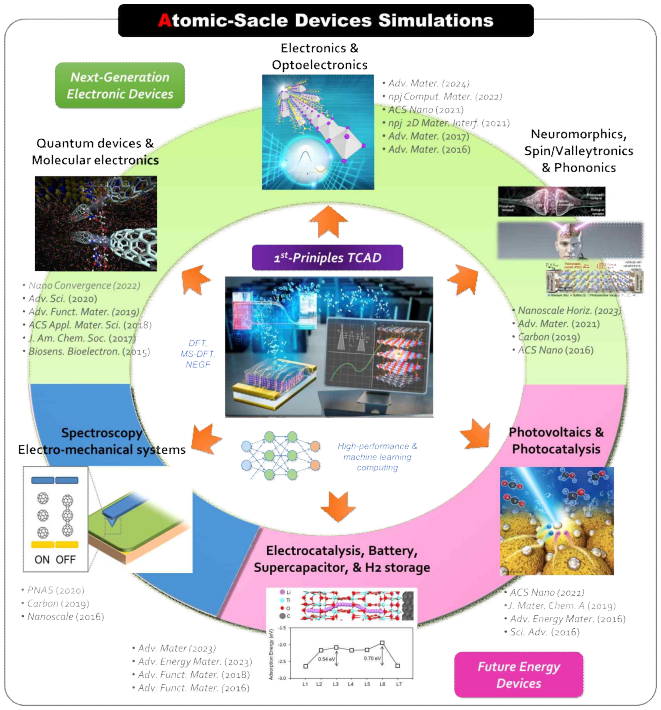
3. More (than) Moore Nano-Devices

- "more Moore (sub-10 nm FET) & more than Moore" devices (multi-value logic, neuromorphic computing.)
- beyond CMOS & quantum technologies
- energy conversion & storage devices (solar cells, LED, electro/photocatalysis, supercapacitor)



■ **Recommended courses & Career after graduation**

- Lab members are expected to have strong interest in (1) advanced (quantum) semiconductor device/process physics, (2) TCAD & high-performance/AI computing
- In the past 5 years, 2 alumni were appointed as an assistant professor; 1 alumnus became permanent staff members in a National Lab; 3 alumni were hired at Samsung as research staff members

■ **Introduction to other activities besides research**

Daedunsan

Jeju island

Barcelona, Spain

- Annual winter schools at ski resorts, Annual summer schools at Jeju, Annual hiking trips, Weekly stroll+lunch
- Regular attendances to International conferences

■ **Introduction to the Lab.**

- Having established the multi-space excitation viewpoint for quantum transport and the multi-space constrained-search density functional theory (MS-DFT) formalism, we are the global leader in the development and application of atomistic TCAD simulations and and their multiscale & AI extensions.
- For the development of "More-Moore" / "More-than-Moore" devices and future quantum technologies, there are currently strong needs to introduce atomic-scale simulation techniques into semiconductor TCAD.
- Atomistic TCAD experts, while their number is very limited, are actively sought after not only by academina but also by the industry leaders like Samsung, Intel, & TSMC.

■ **Recent research achievements ('21~'25)**

- *"Design of Self-Assembled Monolayer in Tungsten Diselenide Bilayer for Exciton Dissociation"*, ACS Nano **19**, 9779 (2025)
- *"Ab initio theory of the nonequilibrium adsorption energy"*, Npj Comput. Mater. **10**, 60 (2024)
- "*High-κ Dielectric (HfO_2)/2D Semiconductor (HfSe2) Gate Stack for Low-Power …*", Adv. Mater. **36**, 2312747 (2024)
- *"Quantum hybridization negative differential resistance from non-toxic halide perovskite …"*, Nano Converg. **9**, 25 (2022)
- *"Gate-versus defect-induced voltage drop and negative differential resistance in vertical …"*, Npj Comput. Mater. **8**, 50 (2022)
- *"An optogenetics-inspired flexible van der Waals optoelectronic synapse and its application …"*, Adv. Mater. **33**, 2102980 (2021)

(23 papers of impact factor > 5 SCI journals in '21-'25; See http://nanocore.kaist.ac.kr for the full publication list)

- Samsung Next Generation ICT Project (2020-2023, http://samsungstf.org) & many other awards on group members.