Hyukjoon Kwon

904-819, Gwanaksa, 599 Gwanak-ro, Gwanak-gu, Seoul, Republic of Korea
+82-10-4213-0327; bagho27@snu.ac.kr;
Website: https://alicism.github.io/

Education

(Master's course) Seoul National University, Seoul, Republic of Korea *Sep 2021 – Present*

(M.S. candidate) Nuclear Engineering
Computational Nuclear Material Laboratory (Supervisor: Takuji Oda)
Academic Concentration: Atomistic Simulation
Relevant Coursework: Path integral molecular dynamics, Forcefield development

(Bachelor's degree) Seoul National University, Seoul, Republic of Korea *Mar 2015 – Aug 2021*

(B.A.) Economics
(B.S.) Nuclear Engineering

Research Experience

Undergraduate Internship Program in Computational Nuclear Material Laboratory *Jul 2020 –Aug 2021*

- Invented efficient algorithms to estimate hydrogen diffusivity in metals including nuclear quantum effects

Joint Development Project of International Thermonuclear Experimental Reactor (ITER) *Mar 2022 – Present*

- Estimated the properties of liquid hydrogen by path integral molecular dynamics.

Joint Research with Samsung Electronics Co., Ltd. *Jun 2022 – Present*

- Developed machine learning potentials on electronics-related metals by active learning.

Publication

(Under review in Acta Materiala) *Sep 2022 – Present*

- Kwon, Hyukjoon and Shiga, Motoyuki and Kimizuka, Hajime and Oda, Takuji, "Accurate Description of Hydrogen Diffusivity in bcc Metals Using Machine-Learning Moment Tensor Potentials and Path-Integral Methods" (October 20, 2022). Available at SSRN: https://ssrn.com/abstract=4254267

Presentations

Japan-Korea Tritium Workshop *Mar 2022*

- Title: *Application of machine learning potential to quantum diffusion of hydrogen isotopes in bcc metal: Machine Learning Path Integral Molecular Dynamics*

Academic Conference of the Korean Institute of Metals and Materials *Apr 2022*

- Title: *Computational analysis on quantum diffusivity of hydrogen in bcc iron: Application of machine learning interatomic potential*

16th International Workshop on Hydrogen Isotopes in Fusion Reactor Materials *Jun 2022*

- Title: *Quantum and isotope effects of hydrogen diffusivity and solubility in bcc metals*

Academic Conference of the Korea Accelerator and Plasma Research Association *July 2022*

- Title: *Analysis on hydrogen diffusivity and solubility in Fe and W by molecular dynamics and machine learning potential model*

Awards

Quantum Information Center Awards (3rd award)
2022 Qhackathon by Ministry of Science and ICT of Korea *Jun 2022*

- Presentation Title: *Analysis on optimal setting for quantum variational eigensolver (QVE)*
- A creative way was suggested to efficiently apply quantum computation for quantum chemistry calculation.

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Academic Interests

- **Path-integral molecular dynamics**
- **Machine learning interatomic potentials**

Technical skills

Computer programming

- Programming Languages: Fortran, C++, python
- Ability to design parallel computation algorithms based on MPI and GPGPU

Atomistic Simulations

- Programs: LAMMPS, VASP, PIMD
- Ability to & modify open source codes (Fortran, C++).

Force Field Development

- Potential models: Embedded Atom Models (EAM), Moment Tensor Potential (MTP)
- Ability to develop machine learning potential for target systems.

Military Service

Korea Army, Republic of Korea
Fire Direction Center (FDC) in Artillery Battalion *Feb 2017 –Nov 2018*

- Honorably Discharged.