# Hyukjoon Kwon

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## Education

### (Master's course) Seoul National University, Seoul, Republic of Korea

Sep 2021 - Present

Department of 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

Bachelor of Economics Bachelor of Nuclear Engineering

## Researach experience

### Laboratory Internship Program in Department of Nuclear Engineering

Jul 2020 -Aug 2021

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

#### Joint Development Project of International Thermalnuclear 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 for electronics-related metals by active learning.

### **Publication**

#### (Under review in Acta Materialia)

Sep 2022 – Present

(1st Author) Accurate description of hydrogen diffusivity in bcc metals using machine-learning moment tensor potentials and path-integral methods

## **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

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

#### 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 Ohackathon 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.

## **Technical skills**

## **Computer programming**

- Programming Languages: Fortran, C++, python
- Ability to design parallel computation algorithms

#### **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.

## **Subjects of Interests**

- Quantum Physics
- Statistical Mechanics
- Materials Science and Engineering
- Computational Chemistry

## **Military Service**

### Korea Army, Republic of Korea

Fire Direction Center (FDC) in Artillery Battalion

• Honorably Discharged.

Feb 2017 -Nov 2018