Cao Thang Nguyen

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EDUCATION

Ph.D. 2/2023	Mechanical Engineering, Ulsan National Institute of Science and Technology (UNIST), South Korea.
M.S. 8/2016	Mechanical Engineering, University of Ulsan, South Korea.
B.S. 5/2010	Mechanical Engineering, HCMC University of Technology and Education, Vietnam.

POSITIONS

2/2023 - present	Postdoctoral Researcher, Ulsan National Institute of Science & Technology (UNIST), South Korea.
3/2017 - 2/2023	Graduate Researcher, Ulsan National Institute of Science & Technology (UNIST), South Korea.
9/2014 - 8/2016	Graduate Researcher, University of Ulsan, Korea.
1/2010 - 9/2014	R&D Staffs, Industrial Zones, Vietnam.

RESEARCH AREAS

- ➢ Computational mechanics and materials science.
- ➢ Structural/crystal elastic instabilities, phase transformation.
- ➢ Atomistic simulations (Molecular Dynamics, Enhanced Sampling, Density Functional Theory)

RESEARCH SKILLS

- ✓ Experienced in **Molecular Dynamics** (MD), **Molecular Statics** (MS) simulations, and transition phenomena simulations. [1–10]
- ✓ Experienced in **Enhanced Sampling** simulations (Steered MD, MetaDynamics, Mean-Force Dynamics, ...) and free energy calculations. [3–5, 10]
- ✓ Experienced in **Thermodynamic Integration (TI)** calculations. [2, 3]
- ✓ Experienced in computational modeling of **2D materials** [4–6], **crystalline** [1–3, 7–10], and **polymeric** [4, 11] molecular systems.
- ✓ Experienced in **compiling** and **running** open-source packages (LAMMPS, PLUMED, OpenMPI, LLVM,...) on high-performance computing (HPC) clusters (example).
- ✓ Experienced in **developing pre- & post-processing codes** [12–23]
- ✓ Experienced in constructing **computational framework** that involves multiple serial/parallel processes on different HPC clusters. [12].
- ✓ Knowledge of application Machine Learning in computational materials science. [5, 12, 14, 17–20]

✓ Knowledge of Density Functional Theory (DFT) calculations.

✓ Knowledge of Finite Element Method (FEM) simulations.

✓ Programming languages: Python, Matlab, C++.

✓ OS: Windows, WindowSubLinux, CentOS, Ubuntu.

✓ Miscellaneous: LAMMPS, PLUMED, GPAW, ASE, DFTD3, OVITO, ABAQUS, SGE, SLURM, GitHub, GitHub-Action, Pip, Conda, Jupyter, Matplotlib, Pandas, Polars, Numpy, Latex, Bibtex, ...

Certificates

2022 Research and Proposal Writing in the Sciences - AuthorAID

2013 SolidWorks Professional in Mechanical Design - Dassault Systems Corp

2012 Hardskills in Project Management - FMIT Institute

PUBLICATIONS

Journal Articles

[1] Cao Thang Nguyen, Duc Tam Ho, and Sung Youb Kim. "Coalescence-enhanced melting in the incipient stage of surface melting". In: *Computational Materials Science* 242 (June 2024), p. 113092. DOI: 10.1016/j.commatsci.2024.113092.

[2] Cao Thang Nguyen, Duc Tam Ho, Viet Hung Ho, and Sung Youb Kim. "Calculation of melting temperature using nonequilibrium thermodynamic integration methods". In: *Advanced Theory and Simulations* (2023), p. 2300588. DOI: 10.1002/adts.202300588.

[3] Cao Thang Nguyen, Duc Tam Ho, and Sung Youb Kim. "An Enhanced Sampling Approach for Computing the Free Energy of Solid Surface and Solid–Liquid Interface". In: *Advanced Theory and Simulations* (2023), p. 2300538. DOI: 10.1002/adts.202300538.

[4] Van Huy Nguyen, Minwook Kim, Cao Thang Nguyen, Muhammad Suleman, Dinh Cong Nguyen, Naila Nasir, Malik Abdul Rehman, Hyun Min Park, Sohee Lee, Sung Youb Kim, Sunil Kumar, and Yongho Seo. "Fast fabrication technique for high-quality van der Waals heterostructures using inert shielding gas environment". In: *Applied Surface Science* 639 (2023), p. 158186. ISSN: 0169-4332. DOI: 10.1016/j.apsusc.2023.158186.

[5] **Viet Hung Ho**, **Cao Thang Nguyen**, **Hoang D. Nguyen**, Hyun Suk Oh, Myoungsu Shin, and Sung Youb Kim. "Hydrogenated Graphene with Tunable Poisson's Ratio Using Machine Learning: Implication for Wearable Devices and Strain Sensors". In: *ACS Applied Nano Materials* 5.8 (2022), pp. 10617–10627. DOI: 10.1021/acsanm.2c01950.

[6] Viet Hung Ho, Duc Tam Ho, Cao Thang Nguyen, and Sung Youb Kim. "Negative out-of-plane Poisson's ratio of bilayer graphane". In: *Nanotechnology* 33.25 (2022), p. 255705. DOI: 10.1088/1361-6528/ac5da0.

[7] **Cao Thang Nguyen**, **Duc Tam Ho**, Seung Tae Choi, Doo-Man Chun, and Sung Youb Kim. "Pattern transformation induced by elastic instability of metallic porous structures". In: *Computational Materials Science* 157 (2019), pp. 17–24. ISSN: 0927-0256. DOI: 10.1016/j.commatsci.2018.10.023.

[8] **Duc Tam Ho**, **Cao Thang Nguyen**, Soon-Yong Kwon, and Sung Youb Kim. "Auxeticity in Metals and Periodic Metallic Porous Structures Induced by Elastic Instabilities". In: *physica status solidi (b)* 256.1 (2019), p. 1800122. DOI: 10.1002/pssb.201800122.

[9] **Duc Tam Ho**, **Cao Thang Nguyen**, Soon-Yong Kwon, and Sung Youb Kim. "Auxeticity in Metals and Periodic Metallic Porous Structures Induced by Elastic Instabilities (Phys. Status Solidi B 1/2019)". In: *physica status solidi (b)* 256.1 (2019), p. 1970010. DOI: 10.1002/pssb.201970010.

*(The authors in **boldface** have equal contributions.)*

Manuscripts

[10] Cao Thang Nguyen and Sung Youb Kim. “Mechanical and thermodynamic melting of metals from the mean-force dynamics calculation”. 2023.

[11] Cao Thang Nguyen and Sung Youb Kim. “Origami-inspired Graphene/PMMA composite with tunable auxetic property”. 2023.

Codes/Tools

[12] Cao Thang Nguyen. *"ALFF: Active Learning Framework for generating Machine Learning Forcefields."*. 2024.

[13] Cao Thang Nguyen. *"thmd: Python package for building models, pre-processing and post-processing Molecular Dynamics simulations."*. 2021.

[14] Cao Thang Nguyen. *"thml: Python package for LLM applications."*. 2023.

[15] Cao Thang Nguyen. *"thutil: Python package for general utilities."*. 2024.

[16] Cao Thang Nguyen. *"molbuilder: Online app to generate models for atomistic simulations"*. 2023.

Open-source contributions

[17] Park et al. “SevenNet: Scalable Parallel Algorithm for Graph Neural Network Interatomic Potentials in Molecular Dynamics Simulations”. In: *Journal of Chemical Theory and Computation* 20.11 (2024). (My contribution: PR#89, PR#92), pp. 4857–4868. ISSN: 1549-9618. DOI: 10.1021/acs.jctc.4c00190.

[18] Batatia et al. *MACE: Higher Order Equivariant Message Passing Neural Networks for Fast and Accurate Force Fields*. (My contribution: PR#586,) Jan. 2023. DOI: 10.48550/arXiv.2206.07697.

[19] Zhang et al. “DP-GEN: A concurrent learning platform for the generation of reliable deep learning based potential energy models”. In: *Computer Physics Communications* 253 (2020). (My contribution: PR#1545, PR#1556, PR#1563, PR#1627), p. 107206. DOI: 10.1016/j.cpc.2020.107206.

[20] Zhang et al. *dpdata is a Python package for manipulating data formats of software in computational science*. (My contribution: PR#614, PR#633). 2020.

[21] Zhang et al. *dpdispatcher is a Python package used to generate HPC (High Performance Computing) scheduler systems jobs input scripts and submit these scripts to HPC systems and poke until they finish*. (My contribution: PR#446, PR#470, PR#473, PR#475, PR#491, PR#501). 2021.

[22] Larsen et al. “ASE: The atomic simulation environment—a Python library for working with atoms”. In: *Journal of Physics: Condensed Matter* 29.27 (June 2017). (My contribution: PR#3529), p. 273002. DOI: 10.1088/1361-648X/aa680e.

[23] Klein et al. “"mBuild: A Hierarchical, Component Based Approach to Screening Properties of Soft Matter"”. In: (2016). (My contribution: PR#1098), pp. 79–92.

Articles in Google Scholar, personal web.

REFEREES

i) Dr. Sung Youb Kim
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ii) Dr. Duc Tam Ho
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