# Curriculum Vitae

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## Work Experience and Education

**BioMap Inc.(Beijing)** **2023.05-Now**

**Westlake University** **2019.03-2023.04**

Research Assistant/postdoc in Biophysics, School of Life Science

**University of Science and Technology of China** **2011.09-2018.06**

Ph. D. in Physics, Condensed Matter Physics, Department of Physics

**Fujian Normal University** **2007.09-2011.06**

B.Sc. in Physics, College of Physics and OptoElectronics Technology

## Research Experience

**Works in BioMap Inc.:**

Physics methods evaluation and exploration of combination with AI models.

**Research Experience in Westlake University:**

MD simulation of biomolecules, Force field development and Biomacromolecules docking.

1. **Protein's Hydrophobicity and Hydrophilicity**

   a) LK repeat peptide's conformation described by Charmm and Drude force field investigated by MD simulation

   b) Study Mechanism of Antifreeze protein by MD simulation

2. **Protein and Small Molecule Force Field Development**

   a) Drude force filed parameter for 19-NT molecule

   b) Integrating HDX-MS experiment data to benchmark and optimize protein force field

3. **Protein/DNA Protein Docking Simulation (Collaborations with experimentalists)**

   a) Receptors/SARS-CoV-2 spike protein docking simulation

   b) HGF/Met and designed ss-DNA/Met docking simulation

   - docking simulation by HADDOCK package to predict the complexes' structure

- estimated binding affinity with MM/PBSA method.

**Research Experience During PhD**:

multiscale simulation and free energy calculations of catalytic reactions on metal/metal nanoparticle surface.

**4. Multiscale Simulation of Nickel Particle Cutting of Graphene**

- MD simulation, DFT calculation and kinetic Monte Carlo simulation were combined together to simulate Ni particle etching graphene.
- metadynamics was used to calculate PMFs of the related processes.

**5. Free Energy Calculation of Methane Dissociation on Cu(111) Surface by AIMD**

- Modifying VASP code to extend its functions in free energy calculation
- Integrating PLUMED package into VASP
- Metadynamics, umbrella sampling and thermodynamics integration method were used to calculate the C-H bond dissociation PMF.

**6. Fitting Si-C System Reactive Force Field Parameters for Simulation of Graphene Epitaxy Growth on SiC at High Temperature**

- Generating database by running MD of SiC surface at 3000K by DFTB+.
- fitting parameters by genetic algorithm.
- Test the generated new parameters set.

**7. Collaborations with Experimentalists**

a) First-principles calculation of $CO_2$ electroreduction to CO by single Ni atoms doped porous carbon nanoparticle.

b) MD simulations of noble gas diffusion and adsorption in water-filled silica nanopore.

## Publication List (co-first author*, correspondence#)


1. S.Wang*, **Z. Qiu***, Y. Hou*, X. Deng*, W., Xu*, Lu Lu#, Jing Huang#, Xu Li# et al, "AXL is a candidate receptor for SARS-CoV-2 that promotes infection of pulmonary and bronchial epithelial cells", *Cell Res. 31,* 126–140 (**2021**)
2. J. Zhang, **Z. Qiu**, Jing Huang#, Zhou Nie# et al, "Scan and Unlock: A programmable DNA molecular automaton for cell-selective activation of ligand-based signaling", *Angew. Chem. Int. Ed. 60*, 6733–6743 (**2021**)
3. X. Zeng*, **Z. Qiu***, Pai Li*, Zhenyu Li# et al, "Steric Hindrance Effect in High-Temperature Reactions", *CCS Chemistry*, *2*, 460-467 (**2020**).
4. Xin Ding#,*, **Z. Qiu*** et al, "Molecular dynamics simulations of noble gas fractionation during diffusion through silica nanopores", *ACS Earth and Space Chemistry*, *3*, 62-69 **(2019)**
5. **Z. Qiu**, Pai Li, Z. Li# and J. Yang, "Atomistic Simulations of Graphene Growth: From Kinetics to Mechanism", *Acc. Chem. Res. 51*, 728-735(**2018**).
6. J. Yang*, **Z. Qiu***, C. Zhao*, Y. Wu#, Z. Li#, et al. "In-situ Thermal atomization to Transfer Supported Metal Nanoparticles to Surface Enriched Ni Single atom catalyst", *Angew. Chem.*

*Int. Ed. 57*, 14095-14100 (**2018**)

7. **Z. Qiu**, S. Li, J. Zhao, Z. Li[#] and J. Yang, "The Nanoparticle Size Effect in Graphene Cutting: A "Pac-Man" Mechanism", *Angew. Chem. Int. Ed. 55*, 9918(**2016**)

## Skills

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|---|---|
| **Software:** | LAMMPS, Charmm, OpenMM, GROMACS, VASP, Gaussian, Material Studio > DFTB+ > CP2K, NWChem；HadDock; |
| **Programing:** | Python, C, Fortran, Shell Script, start to use pytorch recently |
| **Writing:** | Latex, Office |

## Funding

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2020 年浙江省博士后科研项目择优资助，资助编号: ZJ2020077
2021 年杭州市高层次人才特殊支持计划培养类人才