Ye Ding

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Education

Westlake University — Hangzhou
Doctor of Computational Biophysics, School of Life Sciences. — *Sep 2018 – Mar 2024*

Dalian University of Technology — Dalian
Bachelor of Applied Physics, School of Physics. — *Sep 2014 – July 2018*

Projects

DP/MM | *Deep Potential, CHARMM36m, OpenMM, ORCA* — March 2020

- Integrated Deep Potential with the classical force field CHARMM36m to develop the hybrid force field DP/MM, which enhanced the accuracy of atomic forces from MM to QM levels in an **adaptively changing** DP region.
- DP/MM achieves greater **accuracy** than MM and offers more **efficiency** and **flexibility** compared to QM/MM.
- Enhanced the geometry of zinc coordination structures in zinc-protein interactions using DP/MM, achieving significant improvements over traditional MM approaches.

logP Prediction with Drude Force Field | *Drude, logP, FEP, CHARMM* — Dec 2018 – Oct 2019

- Calculated the octanol-water partition coefficient for small molecules by using free energy perturbation (FEP) and the Drude polarizable force field.

Binding Free Energy for Ca^{2+} and Calmodulin EF-Hands | *Drude, CHARMM36m* — Nov 2019 – Oct 2021

- Calculated the absolute binding free energy of Ca^{2+} to Calmodulin EF-hands using the Drude and CHARMM36m force fields.

Experience

Award

- National Scholarship, 2018-2019
- First Class Award of Asia Supercomputer Challenge 2017

DP Technology Research Intern — Aug 2022 - Oct 2022

- Engaged in the development of Induced Fit Docking tools and the deployment.

DP Technology Researcher in CADD — Apr 2024 - Now

- Specializing in advancing Free Energy Perturbation tools, with a focus on implementing Hamiltonian Replica Exchange Molecular Dynamics (H-REMD) and Grand Canonical Monte Carlo (GCMC) methods.

Publications

- **Ye Ding**, Jing Huang et.al, 2020. Predicting partition coefficients of drug-like molecules in the SAMPL6 challenge with Drude polarizable force fields. 10.1007/s10822-020-00282-5
- Qiaozhu Tan, **Ye Ding**, Jing Huang, 2021. Binding Energy and Free Energy of Calcium Ion to Calmodulin EF-Hands with the Drude Polarizable Force Field. 10.1021/acsphyschemau.1c00039
- **Ye Ding**, Kuang Yu, Jing Huang, 2023. Data science techniques in biomolecular force field development. 10.1016/j.sbi.2022.102502
- **Ye Ding**, Jing Huang. DP/MM: A Hybrid Model for Zinc–Protein Interactions in Molecular Dynamics. 10.1021/acs.jpclett.3c03158
- **Ye Ding**, Jing Huang. Implementation and Validation of an OpenMM Plugin for the Deep Potential Representation of Potential Energy. 10.3390/ijms25031448
- Zilin Song, **Ye Ding**, Jing Huang. Constant Advance Replicas Method for Locating Minimum Energy Paths and Transition States. 10.1002/jcc.27178

Technical Skills

Languages: Python, C/C++, CUDA, BASH
Software: OpenMM, DeePMD-kit, CHARMM, ORCA, GROMACS, DMFF, TensorFlow, PyTorch
Developer Tools: Git, VS Code, SLURM, PBS