Gang Huang

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Education

Johannes Gutenberg University of Mainz, Germany

Ph.D., Statistical Physics and Soft Matter

Fields: Statistical Mechanics (Supervisor: Apl. Prof. Dr. M. Sulpizi) Research: Density functional theory(DFT)-based molecular dynamics,

Vibrational sum-frequency generation (VSFG) spectra

Main courses: Ab initio molecular dynamics (Apl. Prof. Dr. M. Sulpizi),

Advanced computer simulations (Dr. H. Behringer, Jun.-Prof. Dr. T. D. Kühne,

Dr. G. Settanni, PD Dr. P. Virnau),

Stochastic thermodynamics (Prof. Dr. T. Speck)

Lanzhou University, Lanzhou, China

M.S., Theoretical Physics, 2008-2011

Main courses: Advanced quantum mechanics (Assoc. Prof. Jie Yang)

Advanced statistical physics (Prof. Lei Tan),

Group theory (Prof. Yuxiao Liu),

Introduction to condensed matter physics (Prof. Honggang Luo),

Quantum field theory (Prof. Jirong Ren),

China West Normal University, Nanchong, China

B.S., Physics, 2004-2008

Main courses: Advanced Mathematics (Prof. Zhonglin Dai)

Atomic physics (Prof. Silin Fan),

Electrical engineering (Prof. Yong Huang)

Electrodynamics (Prof. Zhiquan Luo),

Electromagnetics (Prof. Qiyin Ran),

Experiments of modern physics (Prof. Yong Huang),

Mathematical methods of physics (Prof. Jianshe Peng),

Mechanics (Assoc. Prof. Pingchuan Xu),

Optics (Assoc. Prof. Lijun Liu),

Quantum Mechanics (Prof. Caide Tao),

Theoretical mechanics (Prof. Ruibin Huang)

Thermodynamics and statistical physics (Prof. Silin Fan),

Thermology (Prof. Zhiquan Luo),

Dissertation

Structure, Dynamics and Vibrational Spectroscopy of Interfacial Alkali Nitrate and Alkali Halide Aqueous Solutions from ab initio Molecular Dynamics

Research Institute of Theoretical Physics, Chinese Academy of Sciences (CAS), Beijing, China

Postdoctoral Research Associate, 2019.11-

Project: Hierarchical structure in deep neural networks, (Prof. Yuliang Jin)

Shanghai Institute of Applied Physics, CAS, Shanghai, China

Visiting Scholar, 2015.12-2016.6

Project: Ab initio molecular dynamics and VSFG spectra calculation (Prof. Haiping Fang)

Teaching Institute of Theoretical Physics, CAS, Beijing, China Instructor, Introduction to machine learning, 2019.11

School of Electronic Engineering, Chengdu Technological University, Chengdu, China

Instructor, General physics and experiments, 2017.2-2019.6

Institute for Physics, Johannes Gutenberg University of Mainz, Germany

Teaching Associate, 2013.3-2013.8

DFT and applications (Prof. Dr. M. Sulpizi)

Teaching Associate, 2014.3-2014.8

Quantum field theory (Prof. Dr. H. Meyer)

School of Physics, Lanzhou University, Lanzhou, China

Teaching Associate, Statistical physics (Prof. Lei Tan), 2009.2-2009.7 Teaching Associate, Quantum mechanics (Prof. Lei Tan), 2009.9-2010.1

Awards Excellent Graduate of the Year 2008

School of Physics, China West Normal University, Nanchong, China, 2008.7

Chinese Scholarship Council (CSC) Scholarship

Chinese Scholarship Council, China, 2011.9-2014.9

Recent Publications

- 1. Jie Huang, **Gang Huang***, and Shiben Li*, A machine learning model to classify dynamic processes in liquid water, *ChemPhysChem*, **23**, 42-49, DOI: 10.1002/cphc.202100599, 2022, Cover Article
- 2. Jie Huang, Shiben Li*, Xinghua Zhang*, and **Gang Huang**, Neural Network Model for Structure Factor of Polymer Systems, *The Journal of Chemical Physics*, **153** (12) 124902, DOI:10.1063/5.0022464, 2020
- 3. Xing Liu, **Gang Huang**, Kuan-Kan Hu, Nan Sheng, Chuanshan Tian, Y. Ron Shen, Yu-Chieh Wen, Guosheng Shi*, and Haiping Fang, Sharing of Na⁺ by Three COO⁻ Groups at Deprotonated Carboxyl-Terminated Self-Assembled Monolayer-Charged Aqueous Interface, *J. Phys. Chem. C* **122**, 16, 9111-9116, DOI:10.1021/acs.jpcc.8b02065, 2018

Languages Chinese, English
Skills Python, Fortran
Specific Codes CP2K, LAMMPS
Nationality Chinese



