

Assistant Professor Yunjian Li

Department of Engineering Science, Faculty of Innovation Engineering
Macau University of Science and Technology

Office A305a

E-mail liyunjian@must.edu.mo

Academic Qualification:

Ph.D. in Applied Physics and Materials Engineering, Jun. 2023

Institute of Applied Physics and Materials Engineering, University of Macau, Macao.

B.E. in Road, Bridge, and River-crossing Engineering, Jun. 2020

School of Civil Engineering, Southwest Jiaotong University, Chengdu, China,

Research Area

Ab initio molecular dynamics and enhancing sampling molecular dynamics simulations.

Quantum chemical and density functional theory calculation.

Machine-learning force field development.

Atomistic hydration mechanism of cementitious materials.

Development of new low-carbon cementitious materials.

Academic Publication selected

1. **Y. Li**, H. Pan, Q. Liu, X. Ming, Z. Li*, *Ab initio* mechanism revealing for tricalcium silicate dissolution, **Nature Communications**, 13 (2022) 1253.
2. **Y. Li**, Z. Sun, Z. Li, B. Chen*, Z. Li*, Dimeric and oligomeric interactions between calcium silicate aqua monomers before the calcium silicate hydrate nucleation, **Cement and Concrete Research**, 173 (2023) 107297.
3. **Y. Li**, H. Pan, Z. Li*, Unravelling the dissolution dynamics of silicate minerals by deep learning molecular dynamics simulation: a case of dicalcium silicate, **Cement and Concrete Research**, 165 (2023) 107092.
4. **Y. Li**, H. Pan, Z. Li*, *Ab initio* metadynamics simulations on the formation of calcium silicate aqua complexes prior to the nucleation of calcium silicate hydrate, **Cement and Concrete Research**, 156 (2022) 106767.
5. **Y. Li**, H. Ai, K.H. Lo, Y. Kong, H. Pan*, Z. Li, Insight into adsorption mechanism of water on tricalcium silicate from first-principles calculations, **Cement and Concrete Research**, 152 (2022) 106684.
6. X. Ming, **Y. Li**, Q. Liu, Y. Cai*, Z. Li*, *Ab-initio* modeling of chloride binding at hydrocalumite/sodium chloride solution interfaces, **Cement and Concrete Research**, 156 (2022) 106996.
7. Z. Sun, **Y. Li**, X. Ming, B. Chen*, Z. Li, Enhancing anti-washout behavior of cement paste by polyacrylamide gelation: From floc properties to mechanism, **Cement and Concrete Composite**, 136 (2023) 104887.
8. X. Ming, **Y. Li**, Q. Liu, Y. Cai*, Z. Li*, Chloride binding behaviors and early age hydration of tricalcium aluminate in chloride-containing solutions, **Cement and Concrete Composite**, 137 (2023) 104928.
9. Z. Li, Z. Chen, **Y. Li**, C. Xu Context-aware trajectory prediction for autonomous driving in heterogeneous environments, **Computer-Aided Civil and Infrastructure Engineering**, (2023) 00, 1 – 16.
10. Z. Li, H. Liao, R. Tang, G. Li, **Y. Li**

Research Grant

1. The Science and Technology Development Fund, Macau SAR. “Innovative Processing Technology for Crack-Resistant Concrete”, FDCT-0083/2018/A2, 2019.03-2022.02, Key participant.
2. Multi-Year Research Grant from University of Macau, “Innovative traffic monitoring system with cement-based piezoelectric sensors for smart city”, MYRG2018-00164-IAPME, 2019.01-2021.12, Key participant

Journal Editorship

Invited peer reviewer for Nature Communications.