

## Assistant Professor Yunjian Li

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### 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.