

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/Machine-learning force field/Enhanced sampling molecular dynamics simulation.

Quantum chemical and density functional theory calculation.

Atomistic hydration mechanism of cementitious materials.

Development of new low-carbon cementitious materials.

Academic Publication (selected)

1. **Yunjian Li**, Hui Pan, Qing Liu, Xing Ming, Zongjin Li*, *Ab initio* mechanism revealing for tricalcium silicate dissolution, *Nature Communications* , 13 (2022) 1253.
2. Xing Ming, Wen Si, Qinglu Yu, Zhaoyang Sun, Guotao Qiu, Mingli Cao, **Yunjian Li***, Zongjin Li*, Molecular insight into the initial hydration of tricalcium aluminate, *Nature Communications* , 15 (2024) 2929.
3. **Yunjian Li**, Zhaoyang Sun, Zhenning Li, Binmeng Chen*, Zongjin Li*, Dimeric and oligomeric interactions between calcium silicate aqua monomers before the calcium silicate hydrate nucleation, *Cement and Concrete Research* , 173 (2023) 107297.
4. **Yunjian Li**, Hui Pan, Zongjin 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.
5. **Yunjian Li**, Hui Pan, Zongjin 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.
6. **Yunjian Li**, Haoqiang Ai, Kin Ho Lo, Yongchao Kong, Hui Pan*, Zongjin Li, Insight into adsorption mechanism of water on tricalcium silicate from first-principles calculations, *Cement and Concrete Research* , 152 (2022) 106684.
7. Zhaoyang Sun, **Yunjian Li**, Xing Ming, Qing Liu, Zongjin Li, Binmeng Chen*, Yield stress of in-situ polymerization modified cement paste, *Cement and Concrete Research* , 173 (2023) 107297.
8. Xing Ming, **Yunjian Li**, Qing Liu, Yongqing Cai*, Zongjin Li*, *Ab-initio* modeling of chloride binding at hydrocalumite/sodium chloride solution interfaces, *Cement and Concrete Research* , 156 (2022) 106996.
9. Qing Liu*, Xing Ming, Miaomiao Wang, Qiao Wang, **Yunjian Li**, Zongjin Li, Dongshuai Hou, Guoqing Geng*, Probing the hydration behavior of tricalcium aluminate under the in situ polymerization of acrylic acid, *Cement and Concrete Research* , 177 (2024) 107429.

10. Zhaoyang Sun, **Yunjian Li**, Xing Ming, Binmeng Chen*, Zongjin Li, Enhancing anti-washout behavior of cement paste by polyacrylamide gelation: From floc properties to mechanism, *Cement and Concrete Composite* , 136 (2023) 104887.
11. Xing Ming, **Yunjian Li**, Qing Liu, Yongqing Cai*, Zongjin Li*, Chloride binding behaviors and early age hydration of tricalcium aluminate in chloride-containing solutions, *Cement and Concrete Composite* , 137 (2023) 104928.
12. Yingzi Gu, **Yunjian Li**, Guangxu Ju, Tingyun Zheng, Rui Liang, Guoxing Sun, PCM microcapsules applicable foam to improve the properties of thermal insulation and energy storage for cement-based material, *Construction and Building Materials*, 409 (2023) 134144.
13. Junjie Zhang, Jixin Deng, Yang He, Jiahui Wu, Marta Filipa Simões, Bo Liu, **Yunjian Li**, Shengen Zhang*, André Antunes*, A review of biomineralization in healing concrete: Mechanism, biodiversity, and application, *Science of The Total Environment*, 917 (2024) 170445.
14. Ye Tian, Jiacheng Xu, Xin Xu, Ruoyi Zhao, Guoyi Zhang, **Yunjian Li**, Hongjing Xue, Qing Cai, Jian Cheng, Dongming Yan, Jin Chen, Huzhou Zhu, Xiaojun Luo, Zhiqiang Zhang, Improved magnetic-based apparatus enables non-destructive and high sensitive steel-bar corrosion detection, *Measurement* , 235 (2024) 114930.
15. Ye Tian, Yinzhe Shao, Jiacheng Xu, Ruoyi Zhao, Guoyi Zhang, **Yunjian Li**, Hongjing Xue, Qing Cai, Jian Cheng, Dongming Yan, Jin Chen, Huzhou Zhu, Xiaojun Luo, Zhiqiang Zhang, Bei Li, Developing a Novel Expression for Chloride Ion Concentration Threshold in Reinforced Concrete: Integration of Electrochemical Analysis and Time-Dependent Modeling, *International Journal of Electrochemical Science* , 19, 7 (2024) 100639.
16. Zhenning Li, Zhiwei Chen, **Yunjian Li**, Chengzhong Xu*, Context-aware trajectory prediction for autonomous driving in heterogeneous environments, *Computer-Aided Civil and Infrastructure Engineering* , (2023) 00, 1 – 16.
17. Zhenning Li*, Haicheng Liao, Ruru Tang, Guofa Li, **Yunjian Li**, Chengzhong Xu*, Mitigating the impact of outliers in traffic crash analysis: A robust Bayesian regression approach with application to tunnel crash data, *Accident Analysis & Prevention* , 185 (2023) 107019.
18. Yanchen Guan, Haicheng Liao, Zhenning Li, Jia Hu, Runze Yuan, **Yunjian Li**, Guohui Zhang, Chengzhong Xu, World models for autonomous driving: An initial survey, *IEEE Transactions on Intelligent Vehicles* , (2024) 2379-8904.

Research Grant

1. The Macao Science and Technology Development Fund, Macau SAR. “Development and Application of Water and High-Temperature Resistant Rapid Repair Materials with Magnesium Phosphate Cement”, 0074/2023/RIB3, MOP 953,700, 05/2024 - 05/2026, **Principal Investigator**.
2. The Macao Science and Technology Development Fund and the Ministry of Science and Technology of the People’s Republic of China “Design theory and application technique of recycled concrete in a coastal region” 0096/2023/AFJ, MOP 2,000,000, 01/2024 - 01/2027, **Main Participant**.
3. The Macao Science and Technology Development Fund, Macau SAR. “Development and application of new inorganic multifunctional coatings of heat-insulating, anti-corrosive and anti-fungal magnesium phosphate” FDCT-0147/2022/A3, MOP 1,654,000, 06/2023 - 06/2026, **Main Participant**.
4. Multi-Year Research Grant from University of Macau, “Innovative Traffic Monitoring System with Cement-based Piezoelectric Sensors for Smart City”, MYRG2018-00164-IAPME, MOP 1,500,000, 01/2019 – 12/2021, **Main Participant**.

5. The Macao Science and Technology Development Fund, Macau SAR. “Innovative Processing Technology for Crack-Resistant Concrete”, FDCT-0083/2018/A2, MOP 2,458,000, 03/2019 - 02/2022, **Main Participant.**

Journal Editorship

Invited Reviewer for *Nature Communications* and *Cement and Concrete Research* .