中国科学院武汉岩土力学研究所
Institute of Rock and Soil Mechanics,Chinese Academy of Sciences

岩土力学与工程前沿讲坛

Forum on Geomechanics and Geo-engineering

No.SKL*2025-32*

应岩土力学与工程安全全国重点实验室邀请，香港理工大学 Yong Tao 助理教授来访交流并做学术报告，报告信息如下：

报告人 Lecturer	**Dr. Yong Tao**
讲座题目 Theme	**Atomistic insights into CO2 mineralization with cement minerals**
报告时间 Time	**2025 年 11 月 14 日（周五）上午 10:00**
报告地点 Spot	**武汉岩土所研发大楼 4 楼 1 号会议室**
邀请人 Inv. by	**李江山 研究员　海洋与环境岩土工程研究中心**

欢迎广大科研人员及研究生参加！

岩土力学与工程安全全国重点实验室
State Key Laboratory of Geomechanics and Geotechnical Engineering Safety

中国科学院武汉岩土力学研究所
Institute of Rock and Soil Mechanics,Chinese Academy of Sciences

岩土力学与工程前沿讲坛

Forum on Geomechanics and Geo-engineering

报告简介

While CO_2 mineralization using carbonatable binders and solid waste has become an overwhelming trend in laboratory and industrial trials, a lack of fundamental understanding of the underlying carbonation mechanisms hinders advancement of carbonation technology for large-scale applications. We use Grand Canonical Monte Carlo simulations to unravel the optimal CO_2 sequestration conditions within the mesopores of calcium silicate hydrates. We show that CO_2-surface interactions dominate at low relative humidity (RH), while CO_2-water interactions prevail at high RH, maximizing CO_2 uptake during capillary condensation, where the metastable porewater boosts CO_2 dissolution. We reveal that less hydrophilic minerals require higher optimal carbonation RH. Moreover, using portlandite as an example, we find that the maximum CO_2 intake occurs at an optimal relative humidity (RHopt) when capillary condensation initiates within the hydrophilic mesopores. At this transition state, the pore becomes filled with metastable low-density water, providing an ideal docking site for CO_2 adsorption and forming a mixed metastable state of water/CO_2. We prove that RHopt depends on the mesopore size through a Kelvin-like relationship. Furthermore, we conduct reactive molecular simulations and metadynamics to elucidate the complete interfacial CO_2 mineralization pathways within a portlandite mesopore adsorbed with a nanometric water film. Here we reveal for the first time, a global CO_2 mineralization spectrum describing the local molecular environment and the thermodynamics of the five critical steps: water adsorption, calcium dissolution, CO_2 adsorption, CO_2 speciation, and $CaCO_3$ ion pairing. We identify kinks as the primary reactive sites for surface dissolution and demonstrate how the water film's acid-base environment modulates these processes, creating an energetically favorable reaction loop for sustained CO_2 mineralization.

报告人介绍

Dr. Tao Yong received his joint Ph.D. from Wuhan University of Technology and the University of California, Irvine. He is currently a Research Assistant Professor at The Hong Kong Polytechnic University (PolyU). Dr. Tao is a "Marie Skłodowska-Curie" Fellow, the Young Innovative Researcher Awardee of PolyU, and a member of the Technical Committee of RILEM. He has led/co-led multiple research projects funded by PolyU, the Ministry of Science and Technology of China, the Hong Kong Research Grants Council, and the Innovation and Technology Commission. Dr. Tao's research focuses on cement chemistry, CO_2 mineralization, and atomistic simulations. He has published over 40 papers in top journals including Nature Communications, PNAS, and Advanced Materials. He was awarded the Le Chatelier Distinguished Paper Award from Cement and Concrete Research, and the Excellent Doctoral Dissertation Award from the Chinese Ceramic Society.

岩土力学与工程安全全国重点实验室
State Key Laboratory of Geomechanics and Geotechnical Engineering Safety