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About RILEM

International Union of Laboratories and Experts in Construction Materials, Systems and Structures

国际建筑材料、系统和结构实验室和专家联盟(RILEM)于1947年6月在法国巴黎成立，旨在促进科学合作，促进研究和应用的新方向，从而促进全球建筑领域的卓越发展。

从头算方法揭示硅酸三钙水化与水化硅酸钙形成机理

报告嘉宾 Speaker：李宗津 教授 / **Prof. Zongjin Li**

讲座时间 Time：2022.2.24 (周四) 19:30-20:30 (北京时间)

会议地点 Venue：Zoom ID: 998 1071 7376 (Zoom客户端登陆)
Password: 206 283
请先注册：https://zoom.us/webinar/register/WN_OwlpIGUySNGqzmWGab7qvg

嘉宾介绍 Biography

新的会议系列 “Advanced Materials for Sustainable Infrastructure Development”。李宗津教授现任澳门大学应用物理与材料工程研究院的讲座教授，博士毕业于美国西北大学，为国家973项目“环境友好现代混凝土的基础研究”的首席科学家，共主持科技基金近60项，是国际知名建筑材料专家。曾获美国混凝土学会2017年Arthur R. Anderson 奖章，该奖章由美国混凝土学会董事会根据奖项委员会的建议授予，代表了全球混凝土材料的最高级科研终身成就奖。李宗津教授担任6家国际期刊的编委，美国混凝土学会中国分会的创会主席，国际材料与试验学会（RELIM）中国区分会主席，同时开创了Gordon Research Conference

摘要 Abstract

Understanding the hydration mechanisms of tricalcium silicate (C_3S) and formation process of calcium silicate hydrate (C-S-H) is fundamental in concrete technology, which can help the modification of the materials structure of concrete at nanometer scale and subsequently improving the mechanical properties and durability of concrete. In this study, we provide an exhaustive atomic insight into the C_3S hydration and C-S-H formation by first-principles calculations. First, we introduce the background of C_3S hydration and basic characterization of C-S-H. Then, the adsorption mechanism of water on the C_3S surface is revealed from first-principles calculations. We find the adsorption energy increases with the increase of electron transfer at water/C_3S interface and strength of total Ca-Ow bonds. Next, we discuss the feasibility of the calcium silicate aqua complexes as C-S-H precursors using ab initio metadynamics simulations. We discover two kinds of calcium silicate aqua complexes, $[Ca(H_2O)_n(SiO_2(OH)_2)]$ and $[Ca(H_2O)_n(SiO(OH)_3)]^+$, which have six and five stable states on the free energy surface (FES), respectively and different ligand substitution mechanisms. Moreover, an ab initio mechanism for tricalcium silicate dissolution was unraveled. Finally, the water adsorption, proton exchange and diffusion of water into the surface layer accelerate the leaching of calcium ions from the surface step by step have been investigated.

主办单位：RILEM EAC（国际材料与结构教育发展委员会）
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