



Webinar-43



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Asian Consortium on Computational Materials Science (ACCMS) Global Centre

SRM University-AP, Amaravati

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Screening 2D bilayer structures for photocatalytic and ferroelectric applications using high-throughput DFT calculations, materials genome, and machine learning

Abstract

Two-dimensional (2D) van der Waals (vdW) bilayers have emerged as a rapidly growing frontier in materials research owing to their rich interlayer coupling and potential for next-generation devices. By stacking 2D materials with different configurations, their electronic, structural, and ferroelectric properties can be tailored at the atomic scale. In this talk, I will present our recent progress in combining high-throughput first-principles calculations, materials genome approaches, and machine learning to identify and design vdW bilayers for high-performance photocatalysis and strong out-of-plane ferroelectricity. Starting from our 2D materials database, 2DMatPedia, we systematically explore homobilayer and heterobilayer configurations, focusing on sliding-induced ferroelectricity and photocatalytic water splitting for hydrogen production. Our computational framework screens thousands of bilayer structures and reveals structure–property relationships relevant to experimental realisation. These results demonstrate how high-throughput calculations and data-driven approaches can accelerate the discovery and design of high-performance vdW materials for energy and device applications.

Short Biography

Dr. Lei Shen is a Senior Lecturer in Department of Mechanical Engineering at National University of Singapore (NUS) and NUS Artificial Intelligence Institute. He received his Ph.D. in Physics (2011) from NUS under the supervision of Prof. Yuan-Ping Feng. In 2014, he was awarded the prestigious Lee Kuan Yew Research Fellowship and joined NUS. He currently serves as an Academic Editor for Journal of Materials Informatics and Interdisciplinary Materials. His research focuses on computational materials and device research using first-principles calculations and AI for Science, with interests in 2D materials database development and AI-driven 2D materials discovery and design.



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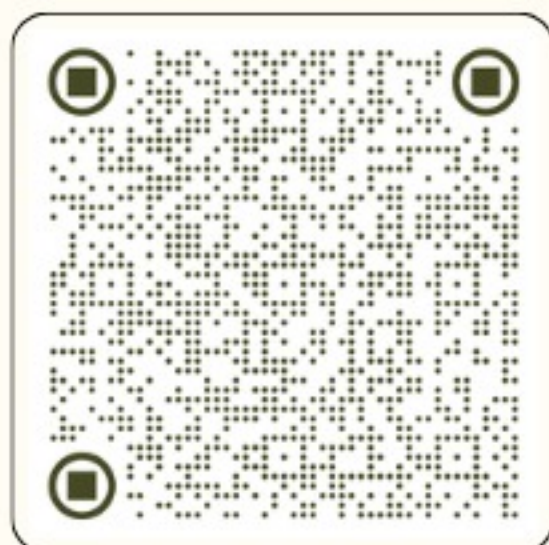


Moderator

Prof. Adisak Boonchun

Associate Professor and Chair
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