GMSI Graduate Program for Mechanical Systems Innovation

CIAiS Research and Education Consortium for Innovation of Advanced Integrated Science

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Materials discovery from first-principles: 1800 novel two-dimensional materials, and what to do next.

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Date: Friday, 26 Oct. 2018, 13:30-14:30
Venue: Faculty of Engineering Bldg. 4, 1F, Room 205

Abstract:

Two-dimensional materials have seen in the past decade very dedicated experimental and theoretical efforts in the quest for novel physics and functionalities. Here, we systematically explore with first-principles calculations known inorganic materials, to identify those that could be exfoliated into two-dimensional layers. We start by curating experimental materials databases, collecting reliable data for 110,000 unique compounds. Then, we identify those that appear layered according to simple geometric and bonding criteria, and launch high-throughput calculations - based on van-der-Waals density-functional theory and 2D density-functional perturbation theory - to characterize binding energies, stability, and properties. Remarkably, we find close to 2000 inorganic compounds that could be exfoliated into novel two-dimensional materials, and recover in the process the known ones - from graphene to transition-metal dichalcogenides to boron nitride and black phosphorus. I'll focus on the exciting properties we are uncovering – with applications ranging from topology to superconductivity, electronics, plasmonics, and catalysis - while highlighting the need for scalable approaches to data and calculations, able to persist and query the full provenance of the calculations, leverage ever growing databases of curated data, and ensure full reproducibility of the workflows.

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