2021 IBS-CALDES Tutorial Lecture

15:00PM, November 12(Fri), 2021

Mechanisms of the bottom-up synthesis of van der Waals materials

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Many emerging technologies call for the controllable fabrication of various van der Waals (vdW) materials. Applications in the semiconducting industry require the synthesis of high-quality vdW materials with a very large, wafer-scale area. To achieve this, a bottom-up synthesis is essential. In this tutorial lecture, I will briefly introduce some parts of more than ten years of our research on mechanisms of the bottom-up synthesis of vdW materials, namely:

i. The intrinsic, weak vdW interaction between a vdW material and the substrate resulting in a new paradigm of materials epitaxy, which is beyond the existing theories of crystal growth. **[1-2]** The development of a theory of vdW materials growth is essential for the controllable synthesis of vdW materials such as large vdW single crystals with desired thickness and twisting angles between neighboring layers as well as for their heteroepitaxial superlattices.

ii. The first example is the mechanism of CVD growth of graphene that includes vdW interaction between graphene and various substrates **[3]**, the mode of graphene CVD growth **[4]**, the alignment of graphene on various substrates **[4]**, and two possible routes towards the synthesis of wafer-scale single crystalline graphene films **[5-7]**.

iii. The second example is the growth mechanism for hexagonal boron nitride (hBN). With the help of our theory **[8]**, we are now able to grow wafer-scale hBN with proper thicknesses **[9]**.

iv. A general theory of vdW materials' epitaxy proposed later **[10]**. Based on a simple analysis, we found that substrates with low symmetry are preferred for the epitaxial growth of various vdW single crystals. The theory is now broadly used to guide the controllable growth of various 2D materials, such as TMDs. **[11-12]**

v. Besides that, I will introduce our experimental efforts on the preparation of high index substrates and on the growth of high-quality graphene which are both assisted by our theoretical studies. **[13]**

I will summarize these achievements, the challenges of the exciting research topics, and the future of vdW materials growth.

References:

[1]. Chem. Rev. 2021, 121, 11, 6321; **[2]** Adv. Mater. 2019, 31, 1801583; **[3]** J. Phys. Chem. Lett. 2012, 3, 2822; **[4]** J. Phys. Chem. Lett. 2014, 5, 3093; **[5]** Adv. Mater. 2015, 27, 1376; **[6]** Nat. Mater. 2016, 15, 43; **[7]** Sci. Bull. 2017, 62, 1074; **[8]** Nanoscale 2017, 9, 3561; **[9]** Nature 2019, 570, 91; **[10]** Nat. Commun. 2020, 11, 5862; **[11]** Nat. Nano., 2021, in press; **[12]** Adv. Funct. Mater. 2021, 31, 2102138; **[13]** Nature 2020, 581, 406.

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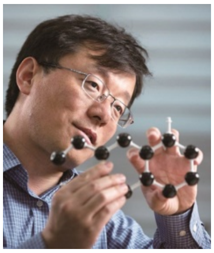
A short biography of the speaker



Prof. Feng Ding received his BS, MS and PhD degrees from Huazhong University of Science and Technology, Fudan University and Nanjing University in 1993, 1996 and 2002, respectively. He is now a Distinguished Professor in Ulsan National Institute of Science and Technology (UNIST) and a Group Leader of the Center of Multidimensional Carbon Materials in the Institute of Basic Science. Prof. Ding's research group focuses on the development of computational methods for materials science applications, theoretical explorations of carbon materials and other 2D materials, especially on their formation mechanisms, the kinetics of their nucleation, growth, and etching.

Prof. Ding coauthored more than 270 SCI papers in leading journals of natural science, including 6 in Nature/Science, more than 20 in sister journals of Nature or Science, more than 50 in PNAS/PRL/JACS/ACIE/AM etc. These publications were cited by more than 16,000 times (Google Scholar). His personal h-index is 69.