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Webinar #7

Prof. Qian Wang

School of Materials Science and Engineering, CAPT, Peking University, Beijing, China

Title: Recent Advances in Pentagon-Based 2D Materials

29th March 2022, 10.00 – 11.30 am IST

Registration link: https://tinyurl.com/4xj8u7c6

Biography

Prof. Qian Wang has received her Ph.D. from Tohoku University (Japan) in 2001. Her research interests are Computational design of new materials with novel properties, Metallicity and Magnetism in carbon-based materials, High energy density materials and materials at high pressure, Electronic structures and magnetic properties of dilute magnetic semiconductors, Inorganic and metal clusters. She has published more than 220+SCI journal papers, including PNAS, Angew. Chem. Int. Ed, JACS, PRL, JPCL, Phys. Rev. B/A, ACS Nano and Nano Lett.; 10+papers are listed as 1% highly cited papers in the Web of Science. 10 of her research works have received media attention, and 12 of her papers have been featured on the covers of journals including PNAS, Angew. Chem. Int. Ed. Nanoscale, ChemPhysChem, Adv. Theory Simul. and J. Chem. Phys.. Her papers have been widely cited in journals. Prof. Wang has been selected in the list of World's Top 2% Scientists for career-long impact. Since 2014, she has been selected among the "Most Cited Chinese Researchers" in Physics & Astronomy every year. Prof. Wang serves as an associate editor for Modern Physics Letters B and International Journal of Modern Physics B, and an editor for MAYFEB Journal of Physics. She is the member of the Editorial Board of several scientific journals. She has received several awards like Xie Xi De Physics Award, ACCMS MID-CAREER AWARD for "Outstanding Scientific Contribution in the Field of Computational Materials Science, and University Award of Teaching Excellence Awards.

Abstract

The most direct and efficient strategy in the design and synthesis of new materials is to change the structural units, which would lead to paradigm shift. Penta-graphene is such an example, where the structural unit is carbon pentagon rather than hexagon as in graphene. Because of its unique geometrical configuration and exceptional properties, penta-graphene has not only received considerable attention, but also becomes a new structural model for other pentagon-based 2D structures. As a result, over 120 nanosheets composed exclusively of pentagon-based structural units have been predicated, as shown in our compiled database for 2D pentagon-based structures (http://www.pubsd.com/). Some of them have been experimentally synthesized, including penta-$PdSe_2$, penta-Si nanoribbons and penta-NiN_2, significantly expanding the family of 2D materials. These pentagon-based 2D materials exhibit interesting physical and chemical properties, including negative Poisson's ratio, intrinsic piezoelectricity, ferromagnetism with high Curie temperature, giant out-of-plane second harmonic generation susceptibility, ferroelasticity, and topological half-metallicity, which provide new insights into problems of technological interest such as metamaterial, piezoelectric conversion, spintronics, battery anode, heterojunctions, water splitting, gas separation, and nano-structured devices. Equally important, the studies on pentagon-based 2D materials have revealed a wealth of information on the structure-property relationships of materials. In this talk, we will briefly discuss the research advances made in this emerging field by focusing on: 1) The classification of all the reported pentagon-based 2D structures based on their geometric characteristics and space groups with emphasizing the role of mathematic models played in new materials design; 2) The main achievements that have provided an in-depth understanding of novel properties, focusing on the intrinsic piezoelectricity; 3) The potential applications of pentagon-based 2D materials, especially, in heterojunctions. The challenges and opportunities in this field will also be discussed.

Zoom meeting details will be shared with the registered participants

Conveners:
Dr. V.J.Surya and Dr.S. Yuvaraj
ACCMS-GRC Center-in-Charges
Department of Physics and Nanotechnology, SRMIST-KTR