NUS National University of Singapore

Department of **Materials Science & Engineering** seminar

Presents

Properties of intrinsic and extrinsic defects in black phosphorus and h-BN

by Prof Alexander Shluger

Date: 16 April 2019 (Tuesday)
Time: 10.30am – 11.30am
Venue: E1-06-03

Abstract

Motivated by perceived applications in 2D nanoelectronics, we investigate the geometric and electronic structures of intrinsic and extrinsic defects in mono- and multilayer black phosphorus (b-P) and hexagonal boron nitride (h-BN) using Density Functional Theory (DFT) and non-local functionals. The results for a monolayer and several layers of b-P demonstrate [1] that energy barriers to forming intrinsic Frenkel pairs and Stone–Wales type defects exceed 3.0 eV and their equilibrium concentrations are likely to be low. P mono-vacancy is shown to introduce a shallow acceptor state in the bandgap of b-P. It exhibits fast hopping rates at room temperature and resulting in coalescence into di-vacancies, thus eliminating the band gap states. Hence P mono-vacancies are not the main contributor to p-doping in b-P with Sn found to be the most promising candidate. Other extrinsic defects considered include I, O, Fe, Cu, Zn and Ni in surface adsorbed, intercalated and substitutional geometries, respectively. Calculations of four-layer slabs of h-BN provide the positions of band boundaries with respect to the vacuum level and positions of charge transition levels for B and N mono- and di-vacancies in the band gap (5.7 eV). The results demonstrate that most of the defects are likely to be charged at typical Fermi level positions. It is found that N-N bridges can be formed between B vacancies in adjacent layers. These results are used to discuss the origins of defect states observed in STM and AFM images of b-P and mechanisms of degradation of h-BN films in devices.

[1] J. Gaberle and A. L. Shluger, *Nanoscale* 10, 19536-19546 (2018)

Speaker

Alexander Shluger graduated from the Latvia State University, Riga, USSR in 1976. He received Ph.D. and Doctor of Science degrees from the L. Karpov Physics and Chemistry Research Institute, Moscow in 1981 and 1988, respectively. He joined the Royal Institution of Great Britain, London in 1991 and the faculty of the University College London in 1996, where he is a Professor of Physics from 2004. He is a Fellow of the Institute of Physics and of the American Physical Society, and a Foreign Member of the Latvian Academy of Sciences. He is a Principal Investigator at the WPI-Advanced Institute of Materials Research, Tohoku University, Japan (from 2007). His current research is focused on theoretical studies of defects in oxides and at semiconductor/oxide interfaces in conjunction with microelectronics applications, the mechanisms of photo-induced processes at oxide surfaces, defects in 2D materials, as well as on modelling of imaging and manipulation of molecules on insulating surfaces using Atomic Force Microscopy.

ALL ARE WELCOME!

Host: A/Prof Michel Bosman