Strain induced superconductivity of Li intercalated bilayer Boron Phosphide by first principles study

Duc-Long Nguyen^{*1,2}, Cheng-Rong Hsing¹, and Ching-Ming Wei¹

¹Institute of Atomic and Molecular Sciences, Academia Sinica (IAMS, Academia Sinica) – No. 1, Roosevelt Rd., Sec. 4, Taipei, 10617, Taiwan

²Department of Physics, National Central University (NCU) – Taoyuan City 32001, Taiwan, Taiwan

Abstract

Monolayer hexagonal Boron phosphide (BP) is a two dimensional narrow direct band gap semiconductor which has an ultra high carrier mobility [1]. Recent experimental and theoretical works show that Li intercalation can induce superconductivity of Black Phosphorous [2] and Graphene [3]. Using first principles calculation, we studied the strain induced superconductivity of Lithium intercalated bilayer BP. From electronic structure, lattice dynamic and electron-phonon coupling calculations, it is suggested that bilayer BP can transform from direct band gap semiconductor to phonon-mediated superconductor under Li intercalated bilayer BP will also be presented. [1] M. Xie, S. Zhang, B. Cai, Z. Zhu, Y. Zou, and H. Zeng, Nanoscale 8, 13407 (2016).

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*Speaker