Electronic and optical properties of monolayer and few-layer films of InSe and GaSe

Vladimir Fal'ko

National Graphene Institute, Manchester, UK

Time: 4:00pm, November 2, 2017 (Thursday)

时间: 2017年11月2日 （周四）下午4:00

Venue: w563, Physics building, Peking University

地点：北京大学物理楼，西563会议室

Abstract

We present the analysis of electronic band structure of InSe and GaSe films, from the stoichiometric mono- to N-layer films, and we describe the resulting optical properties of these 2D materials [1,2] and conduction/valence band parameters. This study is based on the ab initio DFT and related multi-orbital tight-binding model analysis of the electronic band structure and wave functions in the two-dimensional N-layer InSe crystals, and it is compared to the results of luminescence spectroscopy of this material. We show [1-3] that the band gap in InSe (and GaSe) strongly depend on the number of layers, with a strong (more than twice) reduction from the monolayer to crystals with N>6. We find that the conduction-band-edge electron mass in few-layer InSe is quite light (comparable to Si), which suggests opportunities for high-mobility devices and the development of nanocircuits. In contrast, the valence band in mono-, bi- and trilayer InSe is flat, opening possibilities for strongly correlated hole gases in p-doped films. Using the band structure and wave functions, we analyse optical transitions in thin films of InSe, identify their polarisation and compare the results of modelling to the measurements performed on hBN-encapsulated atomically thin InSe crystals.

[1] D. Bandurin, A. Tyurnina, G. Yu, A. Mishchenko, V. Zólyomi, S. Morozov, R. Kumar, R. Gorbachev, Z. Kudrynskyi, S. Pezzini, Z. Kovalyuk, U. Zeitler, K. Novoselov, A. Patanè, L. Eaves, I. Grigorieva, V. Fal'ko, A. Geim, Y. Cao, Nature Nanotechnology 12, 223–227 (2017)
[2]Magorrian, S., Zolyomi, V. & Falko V. , Phys. Rev. B 94, 245431 (2016); V Zolyomi, N Drummond, V.I. Fal'ko, Phys Rev B 89, 205416 (2014); V. Zolyomi, N. Drummond, V.I. Fal'ko, Phys. Rev. B 87, 195403 (2013)
[3] Mudd, G. W., Molas, M. R., Chen, X., Zólyomi, V., Nogajewski, K., Kudrynskyi, Z. R., Kovalyuk, Z. D., Yusa, G., Makarovsky, O., Potemski, M., Fal'ko, V. & Patanè, A., Scientific Reports. 6, 39619 (2016)

About the Speaker

Vladimir Fal'ko is condensed matter theorist responsible for several advances in the theory of electronic and optical properties of atomically thin two-dimensional crystals and fundamentals of nanoelectronics. His current research interests include graphene-based electronic and optoelectronic systems and electronic and optical properties of various atomically thin two-dimensional crystals and their heterostructures. He is one of the initiators of the European Graphene Flagship Project, founder of Graphene Week Conference series and Editor-in-Chief of the IoP Journal '2D Materials'. Falko is currently Director of the National Graphene Institute and Professor of Condensed Matter Theory at the University of Manchester.