Electronic and optical properties of 2D atomic InSe crystals

Vladimir Falko

National Graphene Institute, the University of Manchester, Manchester, UK

We present the analysis of electronic band structure of InSe and (other III-VI semiconductors) films, from the stoichiometric mono-layer to N-layer films, and we describe the resulting optical properties of these 2D materials [1,2]. 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 the variation from 2.7 eV (3.3 eV) in the monolayers to 1.25eV (2 eV) in crystals with N>10. 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 systems

References

[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 (2016); doi:10.1038/nnano.2016.242

[2] Magorrian, S., Zolyomi, V. & Falko V. , Phys. Rev. B 94, 245431 (2016)

[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).