Title: Anomalous optical response in atomically thin InSe

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Indium selenide (InSe) is a layered post-transition metal chalcogenide van der Waals crystal exhibiting a honeycomb in-plane structure that can be exfoliated into a 2D semiconducting crystal of varying thickness. We demonstrate through photoluminescence (PL) measurements that the optical gap of few-layer InSe increases with the reduction of the thickness of the material, and that the principal optical transition vanishes in the monolayer. (See Nature Nanotechnology doi:10.1038/nnano.2016.242 and Scientific Reports 6, 39619 (2016).) We use first principles density functional theory (DFT) to reveal the origin of this anomalous optical behavior, in particular identifying the mirror symmetry of the monolayer as the cause for the vanishing of the principal PL peak. We show that after applying a suitable scissor correction, excitation energies predicted by DFT match the measured PL peak energies of few-layer InSe. We present a tight-binding model parametrized from the scissor-corrected DFT calculations which enables the prediction of the optical transition energies and strengths of multilayer InSe at any thickness. (See Physical Review B 94, 245431 (2016).)

Biography

Viktor Zólyomi obtained his PhD in physics at the Eötvös University in Budapest, Hungary in 2006. He worked as a postdoctoral researcher in Hungary, Austria, and the UK. He won a prestigious Marie Curie Intra-European Fellowship in 2008 and a Marie Curie European (Re)Integration Grant in 2011. He is currently a Research Associate at the National Graphene Institute in Manchester, UK. He has published over 70 scientific papers and earned over 2000 citations to his work with an h-index of 22.

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