Bright and dark excitons and trions in two-dimensional metal dichalcogenides

Vladimir Fal'ko

National Graphene Institute, The University of Manchester, Booth St E, Manchester M13 9PL, UK

We analyse dark and bright states of charged and neutral excitons in two-dimensional transition metal dichalcogenides and metal-chalcogenide semiconductors.

In monolayer transition metal dichalcogenides (TMDC), where both conduction and valence band edges correspond to the Brillouin zone corner, optical spectra affected by the inverted sign of spin-orbit splitting of conduction band states in MoX_2 and WX_2. In WX_2 ground state exciton is dark, whereas the ground state of exciton in $MoSe_2$ is bright. Similarly, trions in $MoSe_2$ are bright, whereas the ground state of the trion in WSe_2 is only weakly radiative (semidark). Also, using diffusion Monte Carlo simulations, we developed interpolation formulae for the exciton and trion binding energies ,taking into account the 2D lattice screening parameter, the electron/hole band masses, and electron-hole exchange.

In monolayer metal dichalcogenides InSe (stoichiometric In_2Se_2) and GaSe, band edges of conduction band and valence band appear near Γ-point, and states have opposite symmetry with respect to $z\rightarrow -z$ mirror reflection, resulting in a weak coupling to the out-of-plane polarised photon. AB stacking of bilayer crystal of InSe (ABC-type for multilayers) violates mirror symmetry, making optical transition with the in-plane polarised light possible, however, only for the excited state of the exciton with angular momentum $|L_z|=1$. To this end, we study the dependence of the gap, effective mass and exciton binding energy on the number of layers. Also, the valence band appears to be quite interesting in all III-VI monolayers and few-layer films: it is almost flat over about 10% of the Brillouin zone area, with a weakly inverted dispersion at the Γ-point, opening possibilities for strongly correlated states of holes in these materials.