Analysis of electronic and optical properties of MoS_2 monolayer and nanostructures using minimal-basis tight-binding model

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Electronic and optical properties of transition metal dichalcogenides (TMDC) monolayer and nanostructures with formula MX_2 are investigated using multi-orbital tight-binding with M d-orbitals and X p-orbitals. TMDC have attracted much attention [1-7] recently due to peculiar optical properties. TMDC monolayers crystallize in two-dimensional honeycomb lattice and harbors a pair of inequivalent valleys in the *k*-space electronic structure, in the vicinities of the vertices of a hexagonal Brillouin zone, ±K points. Exploiting emergent degree of freedom of charge carriers to make 'valleytronics' devices is tempting [8-11].

Ab-initio results show that the conduction band minima (CBM) and valence band maxima (VBM) mostly consist of M d-orbitals [12,13]. Effective two-band (for massive Dirac fermions) and three-band tight-binding models with M d orbitals are widely used [3]. While they properly describe the effects in a vicinity of K points, they may not be sufficient to study optical properties as the second minimum in the conduction band at q-point is not captured.

In this work, we derive 3d-3p band tight-binding model and apply it to study optical properties of one of the transition metal dichalcogenides named MoS_2 monolayer. The nearest (Mo-S) and next nearest (Mo-Mo) neighbor interactions are taken into account. We compare the model with two-band [2] and three-band models [3]. We emphasize important differences and show the role of S p-orbitals. Then, we use it to study the electronic and optical properties of the corresponding nanotubes and nanoribbons. We look at the effects of chirality of nanotubes and nanoribbons on physical properties of MoS_2. The influence of nanotube diameter and width of nanoribbon on electronic and optical properties is shown.

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