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Environment-Dependent Quasiparticle Bandgap of Monolayer MoS_2 YONG-SUNG KIM, Korea Research Institute of Standards and Science, JI-YOUNG NOH, HANCHUL KIM, Sookmyung Women's University, MINKYU PARK, University of Science and Technology, K.C. SANTOSH, K.J. CHO, UT Dallas — 2D semiconductors are manifested by strong Coulomb interaction inside. The strong Coulomb interaction gives remarkable effects on various properties of the 2D semiconductors, including (i) large exciton binding energy (electron-hole), (ii) large quasi-particle self-energy (electron-electron), (iii) large scattering cross section in carrier transports by charged defects (electron-charged defects), (iv) deep defect transition level (bound electron-charged defects), and (v) strong interaction between charged defects (charged defects-charged defects). The ground state, optical, and transport properties are then largely affected by the dielectric environments surrounding the 2D semiconductors, because the Coulomb interaction is effectively screened by the dielectrics. We investigate the electronic band structures of a single-layer MoS2, as a prototype 2D semiconductor, with a variety of dielectric environments by using density-functional-theory (DFT) and GW calculations.

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