First-principles and Quantum-transport Calculations of the Bulk $PtSe_2$/Monolayer $PtSe_2$ Seamless Contact

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Abstract

In this paper, we perform the first-principles and quantum-transport calculations to study the “semiconductive monolayer $PtSe_2$” / “metallic bulk $PtSe_2$” seamless contact. First, we study the interface characteristics of the above semiconductor/metal contact with a 5.5nm-long channel. Second,we use VASP to find the metallization range of the monolayer $PtSe_2$ is about 0.8nm. Third, we simulate the effect of the positive(negative) gate voltage by controlling the band shift through artificially increasing(decreasing) electrons in Nanodcal. Finally, the originally intrinsic channel can be turned into an N(P)-type one. By further comparing the electronic structures and transport properties between the N and P types, we conclude that the former is more advantageous.We also use the Transmission Line Measurement to estimate a contact resistance of about 0.01kΩ·μm.