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Two Strategies to Reduce Contact Resistance between TMDs and Leads: A First Principles Study

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Abstract

Monolayer transition-metal dichalcogenide (TMD) semiconductors are considered candidates for channel materials in next-generation transistors because of their suitable band gaps and high mobilities. However, a high contact resistance between TMDs and conventional metal leads limits the application of the TMDS devices. Some theoretical strategies have been studied to reduce contact resistance and confirmed by Schottky barrier and charge density distribution between channel and leads. Nevertheless, few theoretical researches evaluate the contact resistance by the relation between bias voltage and current density. Furthermore, the current density of industry criterial is 500 micro-Ampere per micro-meter with applying bias voltage 50 millivolts. We suggest two strategies. The T-phase of TMD as a buffer layers or adding halogen atoms between TMDs and metal leads. The phase engineering of two-dimensional TMDs has been studied recently, the phase transition is achieved by several methods. The T phase of monolayer $MoSe_2$ is a semimetal, in contract, the H phase of it is a semiconductor with the band gap 1.7 eV. Meanwhile, the doped halogen atoms may increase carrier density near the fermi level. The quantum transport was applied because the mean free path of an electron is shorter than the length of the channel. The constrained structure relaxation and the electronic structures are executed within the frame work of the DFT. Quantum transport properties were calculated in the frame work of the DFT method, combined with the NEGF as implemented in the Nanodcal package. It calculates the transmission coefficient between two leads. The Landauer's formula is used to calculate the current which is obtained from the transmission coefficient without applying bias and gate voltages. We used a short channel to get the contact resistance in order to exclude a resistance of the semiconductor channel. Our strategy can satisfy the industry's criterial.