Electron Transport through InSe/Metal Heterostructures

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Abstract

The metal-semiconductor contacts are highly concerned in nanoelectronics, and improving the conduction at such atomic interfaces is important for developing such field. Indium Selenide (InSe) has shown its potential for designing 2D heterostructures due to its layer-dependent bandgaps and high carrier mobility, whereas the effects of its contact with different metals are desired to be addressed. Using first-principles calculations based on density functional theory and non-equilibrium Green's function formalism, we investigate the atomic structures and conduction properties of metal (Au, Cu)/InSe interfaces. Particularly, both the atomic structures of InSe edge and the size of overlapped area in-between of metal electrode and the single InSe layer are considered. Our results show that the contact type of InSe/Cu heterostructure is Ohmic, and the contact type of InSe/Au heterostructure is Schottky Contact. It indicates that thin-layered copper is a more suitable material to be the low-resistance 2D contact electrode than thin-layered gold for InSe-based heterojunctions. Additionally, the Schottky barrier heights (SBHs) are higher in InSe/Au series heterojunctions with the zigzag InSe edges at the interface than those with the armchair InSe edges at the interface. The simulated tunnelling barrier heights (TBH) reveals a better strategy to improve the injection efficiency at the contact: Cu > Au, the armchair InSe edge at the interface > the zigzag InSe edge at the interface, and the smaller size of overlapped area is better for the improvement. The calculated conductances, transmission coefficients and average electron densities also indicates that different types of metal, the edge configuration of InSe at the interface and the overlapped size of metal-semiconductor interface are all factors for designing electronic devices.

Keywords - Indium Selenide, 2D Materials, Heterostructures, Quantum Transport, First-principles calculation