ARTICLES

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Bilayer tellurene-metal interfaces

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Abstract: Tellurene, an emerging two-dimensional chain-like semiconductor, stands out for its high switch ratio, carrier mobility and excellent stability in air. Directly contacting the 2D semiconductor materials with metal electrodes is a feasible doping means to inject carriers. However, Schottky barrier often arises at the metal-semiconductors interface, impeding the transport of carriers. Herein, we investigate the interfacial properties of BL tellurene by contacting with various metals including graphene by using *ab initio* calculations and quantum transport simulations. Vertical Schottky barriers take place in Ag, Al, Au and Cu electrodes according to the maintenance of the noncontact tellurene layer band structure. Besides, a p-type vertical Schottky contact is formed due to the van der Waals interaction for graphene electrode. As for the lateral direction, p-type Schottky contacts take shape for bulk metal electrodes (hole Schottky barrier heights (SBHs) ranging from 0.19 to 0.35 eV). Strong Fermi level pinning takes place with a pinning factor of 0.02. Notably, a desirable p-type quasi-Ohmic contact is developed for graphene electrode with a hole SBH of 0.08 eV. Our work sheds light on the interfacial properties of BL tellurene based transistors and could guide the experimental selections on electrodes.

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Supporting Information

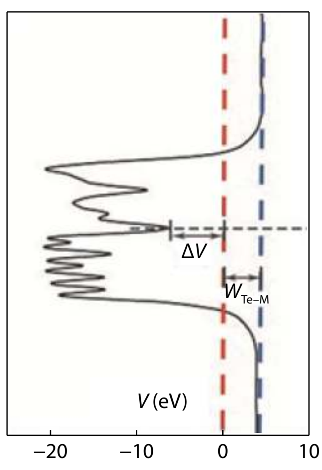

Fig. S1. (Color online) The detailed diagram of the average potential distribution of the Al-BL tellurene system. The red dash line represents the Fermi level and is set to zero. The blue dash line represents the vacuum level, while the black one represents the interface between Al and Te atoms.

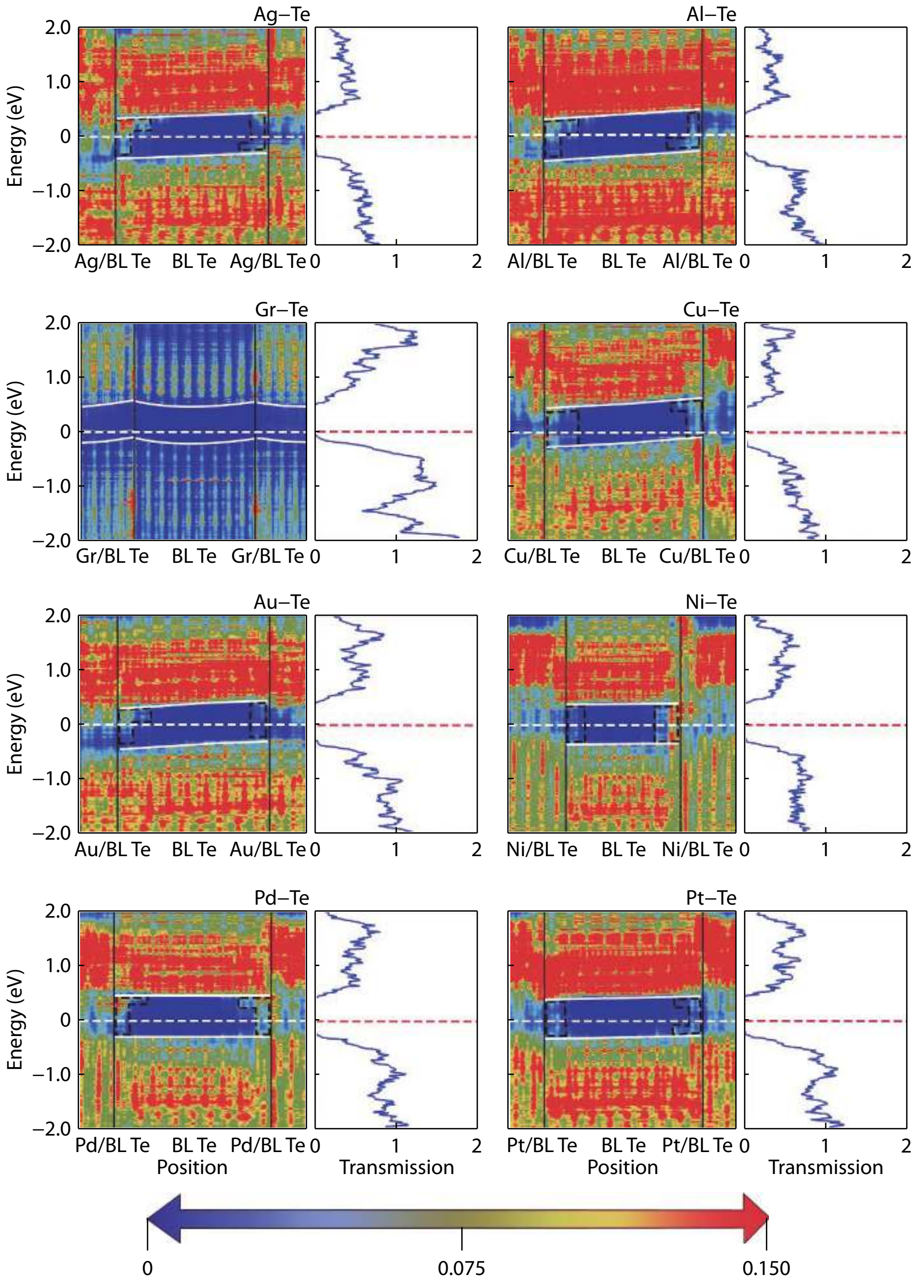

Fig. S2. (Color online) Localized density of states (LDDOS) of the BL tellurene FET devices with metals Al, Ag, Ni, Au, Pd, Pt, Cu and graphene as electrodes (left panel) with a 5-nm channel length as well as the zero-bias transmission spectrum of the FET devices (right panel). The LDDOS is projected to the noncontact tellurene layer. Metal-induced gap states at the interfaces are indicated by the black dashed lines, and the Fermi level is represented by white and red dashed lines.