First-principles calculation of interfacial characteristics between contact metal and two-dimensional materials

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Abstract

According to the literature [1-4], the semimetal contact is believed to be related to better two-dimensional transistor device performance (e.g., higher I_{ON} and lower R_c). Such an explanation can be attributed to the metal-induced gap states (MIGS) effect between contacting interfaces (semimetal contact has a lesser MIGS effect than conventional metal contact). However, our first-principles study showcased that no significant MIGS differences were observed in the semimetal (bismuth, antimony) and conventional metal (gold) contacts. Based on the calculated density of states, van der Waals (vdW) gap distance, and differential charge density, the results indicate that different types of metal contacts primarily influence bandgap shrinkage as well as the location offset between the Fermi level and the conduction band edge; subsequently, lead to variations in interfacial coupling. On the other hand, the strongest interfacial coupling is either found in the near-zero vdW gap metal (Nickel) contact. As a result, we observed that interfacial coupling does not directly correlate with the vdW gap distance. Furthermore, the MIGS effect was not consistently present in every conventional metal contact.

Keywords - first-principles, two-dimensional transistor, metal-induced gap states, van der Waals gap.

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