Motivated by the recent synthesis of the pentagonal PdSe$_2$ sheet [J. Am. Chem. Soc. 2017(139)14090], here using first-principle calculations, we have systematically carried out simulations to investigate the PdSe$_2$ sheet's performance as a channel material when contacted with metal surfaces and graphene. We find that the PdSe$_2$ sheet can almost retain its pentagonal feature with small distortions when contacted with Au(111), Ag(111), Cu(111), and Pb(111) surfaces. However, it is severely distorted on Ti(0001) surface undergoing metallization. Band structure analysis suggests that the vertical Schottky barrier disappears in all of the metal contacts. Au, Ag, Cu, Ti, and Pb are of the Schottky type contacts with barriers of 0.62, 0.87, 0.79, 0.58, and 0.76 eV in the lateral direction for electrons. Whereas both monolayer and bilayer PdSe$_2$ the metal contacts. Au, Ag, Cu, Ti, and Pb are of the Schottky type contacts with barriers of 0.62, 0.87, 0.79, 0.58, and 0.76 eV in the lateral direction for electrons. Whereas both monolayer and bilayer PdSe$_2$ maintain their intrinsic properties when in contact with graphene forming a weak van der Waals interaction with no charge transfer between the two surfaces. Our study provides insight into selecting a high-performance monolayer PdSe$_2$ devices evaluations based on the orbital overlap, tunneling barrier, and Schottky barrier.

**Computational Methods**

- Density functional theory (DFT) calculations: Vienna *Ab initio* Simulation Package (VASP), projector augmented wave (PAW) method with plane wave basis set, GGA-PBE functional, HSE06 functional for electronic structure calculations
- Electrical polarization calculations: Berry phase method
- The energy cutoff is set at 500 eV
- The convergence criteria for energy and force are set to 0.0001 eV and 0.01 eV/Å, respectively.

**Results and Discussion**

- Geometry and Computational Models

  - Electrostatic potential along the z direction:
  - The tunneling barrier is obvious in PdSe$_2$/Au, Ag and Pb contacts
  - The tunneling barrier is obvious in PdSe$_2$/Au, Ag and Pb contacts