Abstract

High-performance electronic and optoelectronic devices rely heavily on efficient charge transport at material interfaces. This study investigates critical factors influencing contact resistance in 2D-semiconductor/metal contacts through computational modeling. We focus on two promising 2D semiconductors: phosphorene and transition metal dichalcogenide (WS_2). A comprehensive analysis of 18 different metal electrodes (Ag, Al, Au, Co, Cr, Cu, Mo, Nb, Ni, Pd, Pt, Ru, Sc, Ta, Ti, W, V, and Zn) for phosphorene reveals the interplay between mechanical and electrical properties at the interface. This broad exploration allows for identifying optimal electrode materials that minimize contact resistance. For WS_2, we strategically downselected six metals (Ag, Au, Cu, Pd, Pt, and Sc) with varying electronegativity and work function. This targeted approach ensures a thorough understanding of the mechanical and electrical behavior of WS_2/metal interfaces while maintaining applicability to diverse contact scenarios. Building upon established knowledge, we further explored the potential of substitutional dopants (C, Cl, P, N, O, and F) in WS_2 to enhance contact properties. Our investigation evaluates several interface properties for their effectiveness in reducing contact resistance and ultimately achieving superior performance in 2D semiconductor devices. Notably, our study reveals that metal selection can be a feasible approach for phosphorene-based contacts, while for WS_2, C, P, and N-doping can lead to reduction in Fermi level pinning (FLP), a highly desirable outcome, without compromising the mechanical stability of the interface. At the same time, Cl and F-dopants can provide a path to lower the n-type Schottky barrier height (SBH). Our method provides an alternative approach to reduce the FLP that doesn't increase the tunneling barriers, which is not observed with other interface engineering methods. This work can guide further experimental work in designing and accelerating the discovery of optimal and low-energy consuming 2D-semiconductor/metal interfaces.

Keywords: *Schottky barrier*, *ab initio*, *Phosphorene*, *WS_2*, *semiconductor-metal interface*, *Tunnel barrier*, *metal-induced gap states*, *Fermi level pinning*, *Contact resistance*, *Interface dipole formation*