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Design of low work function materials using alkali metal-doped transition metal dichalcogenides SOL KIM, Pohang Univ of Sci Tech, MAN YOUNG LEE, SEONG LEE, 4th RD Institute-4, Agency for Defense Development., SEUNG-HOON JHI, Pohang Univ of Sci Tech — Engineering the work function is a key issue in surface science. Particularly, discovering the materials that have work functions less than 1eV is essential for efficient thermionic energy conversion. The lowest work function of materials, reported so far, is in a range of about 1eV. To design low work function materials, we chose MX_2 (M=Mo and W; X=S, Se and Te) as substrates and alkali metals (Li, Na, K, Rb and Cs) as dopants, and studied their electronic structures, charge transfer, induced surface dipole moment, and work function using first-principles calculations. We found that the charge transfer from alkali metals to MX_2 substrates decreases as the atomic radius of alkali metals increases. Regardless of the amount of the charge transfer, K on WTe_2 exhibits the biggest surface dipole moment, which consequently makes the surface work function the lowest. Also, we found a correlation between the binding distance and the work function.

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