ST-P010

Contribution of van der Waals Interactions to the Adsorption Energy of C_2H_2, C_2H_4, and C_6H_6on Si(100)

김선우, 이준호, 조준형

한양대학교 물리학과

Usingvan der Waals (vdW) energy-corrected density-functional theory without or with self-consistent screening (SCS) effects, we calculate the adsorption energy of acetylene, ethylene and benzene on Si(100). We find that vdW interactions without SCS effects increase the adsorption energy by 0.23, 0.30, and 0.64 eV for adsorbed C_2H_2, C_2H_4, and C_6H_6 on Si(100), respectively. However, if SCS effects are included, this increase of the adsorption energy is reduced as 0.19, 0.24, and 0.54 eV for the three adsorption systems, respectively. The resulting adsorption energy for each system is between the values computed using the local-density approximation and the generalized-gradient approximation.

Keywords: Van der Waals interactions acetylene, Ethylene, and benzene with Si(100)