Large Enhancement and Tunable Band Gap in Silicene by Small Organic Molecule Adsorption

T. P. Kaloni, G. Schreckenbach, and M. S. Freund

Department of Chemistry, University of Manitoba, Winnipeg, MB R3T 2N2, Canada

Abstract

Adsorption of eight organic molecules (acetone, acetonitrile, ammonia, benzene, methane, methanol, ethanol, and toluene) onto silicene has been investigated using van der Waals density functional theory calculations (DFT-D). The calculated values of the adsorption energies vary from −0.11 to −0.95 eV. Quantitatively, these values are higher than the corresponding adsorption energies of the molecules adsorbed on graphene. In addition, electronic structure calculations have been performed. The obtained values of the band gap range from 0.006 to 0.35 eV for acetonitrile to acetone, respectively. Furthermore, the effective mass of the electron is estimated and found to be comparatively small, which is expected to result in high electron mobility. In addition, we study the effect of Li atoms doped in pristine and acetone adsorbed silicene. In particular, we focus on the variation of the adsorption energy with respect to the number of Li atoms in the systems. Our results suggest new approaches for the use of silicene molecular-based energy storage and conversion as well as electronic devices.

Reference: T. P. Kaloni, G. Schreckenbach, and M. S. Freund, J. Phys. Chem. C, 118, 23361 (2014).