

CHAPTER IV

Conclusions

In conclusion, we investigated the capability of silicene-based devices for sensing chemical gases in terms of sensitivity and selectivity. We employed first-principles electronic structure calculations based on density functional theory formalism. For adsorption of NO, NO₂, NH₃ and CO on pristine (P-), B-doped or N-doped silicene, we determine the adsorption configurations, binding energies, charge transfer and change in the electronic transport properties. Our results reveal that P-silicene can detect NO and NO₂ gas molecules with high sensitivity. However, this is limited to CO and NH₃ due to weak van der Waals interaction between those gases and P-silicene. By doping P-silicene with either B or N atoms, enhanced binding and charge transfer of all studied gases on the nanosensor were achieved, resulting in an increased sensitivity towards NH₃ and CO detection. However, doped-silicene strongly bound to NO and NO₂ is not presumably suitable for practical gas sensor devices. Based on our results, we can conclude that by doping with different impurities, one can create a silicene device that is able to detect different gas species with high sensitivity and selectivity.