Theoretical Study of Dopamine Sensing on Semiconducting Single-Walled Carbon Nanotubes

Wan-Ru Shie, Yung-Jou Hsiao, Chen-Hao Yeh and Jyh-Chiang Jiang *

Department of Chemical Engineering, National Taiwan University of Science and Technology, Taipei, Taiwan, R.O.C

Dopamine(DA) is one of the catecholamine neurotransmitters which can cause some nervous system disorders resulting in Parkinson's disease. Thus, the development of dopamine sensor is important for the diagnosis of these disorders. In this work, the sensing mechanism of dopamine (DA) on semiconducting boron-nitrogen codoped (6,5) single-walled carbon nanotube based sensor has been investigated by DFT calculation. The results reveal that there is the large conductivity change on 0.55% B-N codoped (6,5) SWNT and 2.20% B-N codoped (6,5) SWNT after the adsorption of neutral DA owing to strong dative bond between nitrogen atom of DA and the boron atom of SWNT and the C-H$\cdots\pi$ interaction between DA and SWNT. Moreover, as the doping concentration being smaller than 4%, the B-N codoped (6,5) SWNT is suitable to be a conducting sensor due to the large conductivity change. In contract, as the doping concentration being larger than 4%, the B-N codoped (6,5) SWNT tends to be a resistive sensor. As a result, our calculated results indicate that B-N codoped (6,5) SWNTs display high sensitivity toward to the DA detection and sensing.

Email: jcjiang@mail.ntust.edu.tw