Optical fingerprints and electron transport properties of DNA bases adsorbed on monolayer MoS_2

Munish Sharma[a], Ashok Kumar[b] and P. K. Ahluwalia[a]

[a]Department of Physics, Himachal Pradesh University, Shimla 171005, India.
[b]Centre for Physical Sciences, School of Basic and Applied Sciences, Central University of Punjab, Bathinda, 151001, India
munishsharmahpu@live.com

Abstract Electronic, optical and transport properties of DNA nucleobase adsorbed on monolayer MoS_2 has been investigated using density functional theory. A significant polarization in MoS_2 has been observed upon DNA nucleobase adsorption. The nucleobase origin of the modulation in the electronic properties is clearly captured in the simulated STM measurements (figure 1). The electronic transport through conjugate systems allows the clear distinction of nucleobase from one another. The modulation in electron energy loss spectra and transport properties of pristine MoS_2 has been observed on nucleobase adsorption which could serve as a fingerprint for realization of next generation DNA sequencing devices. We believe that these results also bring out the possibility of fabrication of MoS_2 based biosensors for selective detection of DNA bases in real long-chain DNA molecules.

References

[1] T. Ahmed, S. Kilina, T. Das, J. T. Haraldsen, J. J. Rehr and A. V. Balatsky, Nano Lett., **12** (2012) 927
[2] S. Gowtham, R. H. Scheicher, R. Pandey, S. P. Karna and R. Ahuja, Nanotechnology, **19** (2008) 125701
[3] T. Kuila, S. Bose, P. Khanra, A. K. Mishra, N. H. Kim and J. H. Lee, Biosens. Bioelectron, **26** (2011) 4637
[4] Y. Shao, J. Wang, H. Wu, J. Liu, I. A. Aksay and Y. Lin, Electroanalysis, **22** (2010) 1027
[5] C. Sathe, X. Zou, J.-P. Leburton and K. Schulten, ACS Nano, **5** (2011) 8842
[6] S. Meng, P. Maragakis, C. Papaloukas and E. Kaxiras, Nano Lett., **7** (2007) 45
[7] M. Sharma, A. Kumar, P. Ahluwalia and R. Pandey, J. Appl. Phys., **116** (2014) 063711.
[8] D. Sarkar, W. Liu, X. Xie, A. C. Anselmo, S. Mitragotri and K. Banerjee, ACS Nano, **8**, (2014) 3992
[9] X. Gan and H. Zhao, Sens. Mater., **27** (2015), 191
[10] R. G. Amorim and R. H. Scheicher, Nanotechnology, **26**, (2015), 154002.

Figures

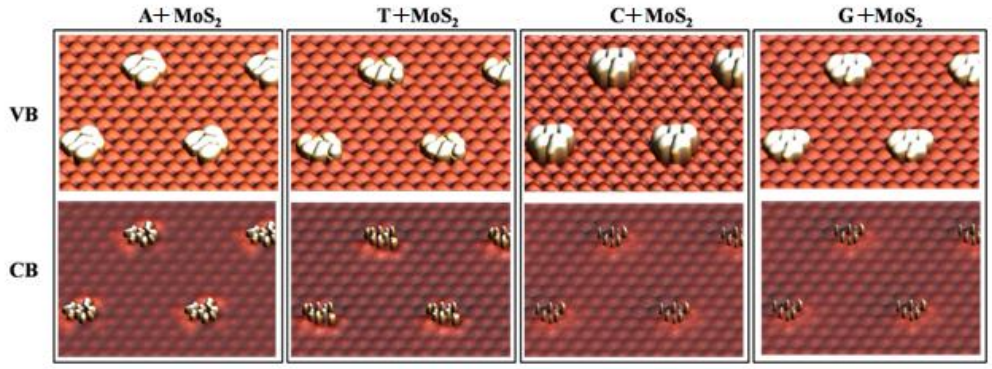

Figure 1: Simulated STM-like topographical images of DNA nucleobase adsorbed on MoS_2 for valance band (VB) and conduction band (CB) at biasing of ±1.5 eV between sample and Tip.