First Principles Study on Optical Properties of Monolayer Bismuthene under an Electric Field

W. C. Liu,[1] L. L. Xu,[1] M. C. Lin,[1] T. C. Leung,[2] H. Y. Hsu,[3]

[1] *Multidisciplinary Computational Laboratory, Department of Electrical and Biomedical Engineering, Hanyang University Seoul 04763, South Korea*

[2] *Department of Physics, National Chung Cheng University, Chia-Yi 62101, Taiwan, Republic of China*

[3] *Department of Mechanical Engineering, National Taipei University of Technology, Taipei 10608, Taiwan, Republic of China*

Monolayer bismuthene has extraordinary optoelectronics, catalytic and biocompatible properties, and potential as a 2D topological insulator. When monolayer bismuthene is deposited in a sufficiently thin layer on an object, it possesses a stable low-buckled hexagonal structure and it has the property of semiconducting, which could be a promising low-dimensional thermoelectric material. Monolayers bismuthene is p-type semiconductors, but the hole concentration arising from the intrinsic defects is very low and hard to control. In this work, the band structure, density of states and optical constant of monolayer bismuthene have been calculated using first-principle calculations based on density functional theory (DFT). The results are compared to those calculated from the tight-binding model. With an applied external electric field, it is found that the electric and optical properties will be dramatically changed. Monolayer bismuthene can be calculated may generate some applications in optoelectronics, either combined with other 2D materials or topological materials.

[1] R. B. Chen, D. J. Jang, M. C. Lin, and M. F. Lin, Opt. Lett. **43**, 6089 (2018).

[2] F. F. Xia, S. Y. Xiong, Y. Y. He, Z. B. Shao, X. J. Zhang, and J. S. Jie, J. Phys. Chem. C 2017, **121**, 19530-19537.

[+] Author for correspondence: ***mclin@hanyang.ac.kr***