

First principles study on electronic properties of graphene nanostructures for high current density cathode

N. Zhao,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*

Graphene is a crystalline allotrope of carbon with two-dimensional properties. Its carbon atoms are densely packed in a nano-scale hexagonal pattern. Graphene has many unusual properties. It is about 200 times stronger than the strongest steel. It can efficiently conduct heat and electricity and is nearly transparent. In this work, we study the electronic properties of graphene using first principles or *ab initio* calculations based on density functional theory (DFT) in order to explore its applications in field emission devices. The change of work function due to the lattice deformation of graphene is investigated using a supercell including a vacuum layer which is thick enough so that the layer interaction is negligible. It is found that the work function is very sensitive to the lattice size. As the lattice site increases, the work function increases proportionally. However, the work function is reduced doubly while the lattice site is reduced. The local work function of graphene has also been determined and this can be used to predict field emission current from Fowler-Nordheim equation more accurately. For realistic applications, this approach has been used to calculate the work function of carbon nanoribbons with different widths and terminating edges with and without passivation.

- [1] D. W. Boukhvalov, M. I. Katsnelson, and A. I. Lichtenstein, "Hydrogen on graphene: Electronic structure, total energy, structural distortions and magnetism from first-principles calculations", *Phys. Rev. B* 77, 035427 (2008)
- [2] D. R. Cooper, B. D'Anjou, N. Ghattamaneni, B. Harack, M. Hilke, A. Horth, N. Majlis, M. Massicotte, L. Vandsburger, E. Whiteway, and V. Yu, "Experimental Review of Graphene", *ISRN Phys. Condens. Matter.* 2012, 501686 (2012).
- [3] V. Meunier, A. G. Souza Filho, E. B. Barros, and M. S. Dresselhaus, "Physical properties of low-dimensional sp²-based carbon nanostructures", *Rev. Mod. Phys.* 88, 025005 (2016).
- [4] D. G. Kvashnin, P. B. Sorokin, J. W. Brünig, and L. A. Chernozatonskii, "The impact of edges and dopants on the work function of graphene nanostructures: The way to high electronic emission from pure carbon medium", *Appl. Phys. Lett.* 102, 183112 (2013).
- [5] T. C. Leung, C. L. Kao, W. S. Su, Y. J. Feng and C. T. Chan, "Relationship between surface dipole, work function and charge transfer: to an established rule" , *Phys. Rev. B* 68, 195408 (2003).

⁺ Author for correspondence: mclin@hanyang.ac.kr