

Nanoroads and quantum dots on fluorinated graphene

Ribas M.A.¹, Singh A.K.², Sorokin P.B.^{*3}, Yakobson B.I.¹

¹Rice University, 77005, Houston, Texas, USA

²Materials Research Centre Indian Institute of Science 560012, Bangalore, India

³Technological Institute for Superhard and Novel Carbon Materials,
142190 Troitsk, Moscow region, Russian Federation

*e-mail: PBSorokin@gmail.com

After the first experimental evidence of graphene research on its properties and applications has continued to grow with unprecedented pace. However, a lot remains to be done to fully incorporate graphene's unique properties into electronic devices. The quick advances on fabrication methods have now made it possible to produce graphene in larger scale. The major hurdle for its application in electronic devices is the lack of a consistent method to open the zero gap of graphene in a controlled fashion.

A recently proposed alternative [1] to open the zero-gap is to use a fully hydrogenated graphene (also known as graphane) as a matrix where graphene nanoroads or dots are patterned. The biggest advantage over the nanoribbons is that both semiconducting and metallic elements can be patterned on the same graphene sheet. The nanoroads and quantum dots can be patterned on any insulating functionalized graphene, e.g., graphane. Here we explore the functionalization of graphene by fluorine which was released experimentally quite recently [2].

Using *ab initio* methods we investigate the fluorination of graphene and find that a complete CF phase can be formed without any nucleation barrier. The fluorinated graphene is an insulator and turns out to be a perfect host for patterning nanoroads and quantum dots of graphene. Depending upon the edge orientation and width the electronic and magnetic properties of the nanoroads can be tuned. The energy gap between the highest occupied and lowest unoccupied molecular orbitals (HOMO-LUMO) of quantum dots are size dependent and show a typical confinement of Dirac fermions. Furthermore, we study the effect of different coverages of F on graphene on their band gaps, and show their suitability to host quantum dots of graphene with unique electronic properties.

- [1] A.K. Singh, B.I. Yakobson, *Nano Lett.* **9**, 1540 (2009); L.A. Chernozatonskii, P.B. Sorokin and J. Brünig, *Applied Physics Letters* **91**, 183103 (2007)
- [2] R.R. Nair, W. Ren, R. Jalil, I. Riaz, V.G. Kravets, L. Britnell, P. Blake, F. Schedin, A.S. Mayorov, S. Yuan, M.I. Katsnelson, H.M. Cheng, W. Strupinski, L.G. Bulusheva, A.V. Okotrub, I.V. Grigorieva, A.N. Grigorenko, K.S. Novoselov, A.K. Geim, *Small* **6**, 2877 (2010); S.H. Cheng, K. Zou, F. Okino, H.R. Gutierrez, A. Gupta, N. Shen, P.C. Eklund, J.O. Sofo, J. Zhu, *Phys. Rev. B* **81**, 205435 (2010); J.T. Robinson, J.S. Burgess, C. Junkermeier, S.C. Badescu, T.L. Reinecke, F.K. Perkins, M.K. Zalalutdniov, J.W. Baldwin, J.C. Culbertson, P.E. Sheehan, E.S. Snow, *Nano Lett.* **10**, 3001 (2010).