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Electronic structure and energetics of graphene antidot lattice MASAHIRO SAKURAI, Institute for Solid State Physics, University of Tokyo, SUSUMU SAITO, Department of Physics, Tokyo Institute of Technology, YASUTAMI TAKADA, Institute for Solid State Physics, University of Tokyo — We have made a systematic study of the electronic structure and the energetics of graphene with periodic array of vacancy clusters (graphene antidot lattice) in the framework of the density-functional theory (DFT). We find that the electronic property of the system is well controlled by its lattice periodicity. More specifically, this system can be either metallic or semiconducting, depending on its lattice geometry. Interestingly, some of them are predicted to be direct-gap semiconductors. For example, graphene sheet with high-symmetry arrangements of periodic circle-shape vacancies always has a direct fundamental gap [1]. The DFT total-energy calculations indicate that the geometry of hole edges plays an important role in determining its stability. [1] "Electronic properties of graphene and boron-nitride based nanostructured materials" M. Sakurai, Y. Sakai, and S. Saito, J. Phys.: Conf. Ser. 302 (2011) 012018.

Masahiro Sakurai
Institute for Solid State Physics, University of Tokyo

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