Holes in graphene

Graphene antidot lattices on metal surfaces

B. Paulus, J. Shao, Institut für Chemie und Biochemie, Freie Universität Berlin substrate interactions. Herein, we investigate the effect of different metal substrates on the properties

In Short

- Exploring the formation of graphene antidot lattices on metal surfaces.
- How do different metals influence the properties of graphene antidot lattices?

Graphene, a 2D form of carbon, has seen enormous interest over recent years, attracting the attention of experimental and theoretical researchers alike [1]. Its high mechanical and chemical stability, combined with exceptional electronic as well as thermal conductance, make graphene a natural candidate for use in high-performance transistor technology. The realization of practical devices is though made difficult by the absence of an electronic band gap. A number of different ways have been proposed to overcome this problem, ranging from its deposition on substrates breaking the sublattice symmetry [2] to its chemical functionalization [3], and we ourselves have in the past investigated a number of these structures [4-6]. Another method of modifying the electronic properties of graphene, while at the same time maintaining many of its attractive properties, consists in the introduction of holes into the graphene lattice. Structures in which the arrangement of such holes is well-defined periodically, are referred to as graphene antidot lattices (GALs) and show a number of interesting properties such as a finite band gap, controllable via the size of the holes in the GALs [7]. An example of this type of lattice is shown in fig. 1.

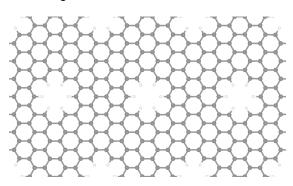


Figure 1: Example of a graphene antidot lattice.

While the effect of the sizes and periodic arrangement of holes on GALs has been widely discussed in the literature, little is known about the effect of substrate interactions. Herein, we investigate the effect of different metal substrates on the properties of a number of GALs of varying structure. To this end we first employ vdW-DFT to accurately account for the weak interactions between the substrate and the adsorbed layer. We then employ recently developed methods to incorporate screening effects within vdW-bound systems [8] to study the effects of metal adsorption on the electronic structure of the GALs within the G_0W_0 approximation.

www

http://www.bcp.fu-berlin.de/chemie/

More Information

- A. K. Geim, K. S. Novoselov, and S. Konstantin, *Nat. Mater.* 6, 3 (2007). doi:10.1038/nmat1849
- [2] G. Giovannetti, P. A. Khomyakov, G. Brocks, P. J. Kelly, J. Paul, and J. Van Den Brink, *Phys. Rev. B* **76**, 7 (2007). doi:10.1103/Phys-RevB.76.073103
- [3] T. Kuilaa, S. Bosea, A. Kumar Mishrab, P. Khanraa, N. Hoon Kimc, and K. Hee Lee, *Prog. Mater. Sci.* 57,7 (2012). doi: 10.1016/j.pmatsci.2012.03.002
- [4] L. E. Marsoner Steinkasserer, N. Gaston, and B. Paulus, *J. Chem. Phys.* **142**, 15 (2015). doi: 10.1063/1.491717
- [5] L. E. Marsoner Steinkasserer, A. Zarantonello, and B. Paulus, *Phys. Chem. Chem. Phys.* 18, 36 (2016). doi:10.1039/C6CP05188J
- [6] L. E. Marsoner Steinkasserer and B. Paulus, *ArXiv* arXiv:1703.08582 (2017).
- [7] J. A. Fürst, J. G, Pedersen, C. Flindt, N. A. Mortensen, M. Brandbyge, T. G. Pedersen, and A.-P. Jauho, *New J. Phys.* **11**, 9 (2009). doi:10.1088/1367-2630/11/9/095020
- [8] K. T. Winther and K. S. Thygesen, 2D Mater. 4, 2 (2017). doi:10.1088/2053-1583/aa6531

Funding

DFG Schwerpunktprogramm 1459 "Graphene" Studienstiftung des deutschen Volkes IMPRS Complex Surfaces in Material Science