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Graphene revisited: From orbital mapping to its impact as a substrate[1]

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Graphene, the material of the 21st century, is without doubt one of the best characterized solids. Despite the enormous amount of investigations and related publications, it still it offers a variety of exciting aspects to explore, in particular in view of its excitations. Combining density-functional theory with many-body perturbation theory, as implemented in the all-electron full-potential package **exciting** [1], provides a powerful framework for this purpose. (i) The first example concerns the question, whether we can "see" orbitals in an electron microscope. Indeed, transmission electron microscopy can be used for mapping atomic orbitals, as demonstrated recently by a first-principles approach [2]. For defected graphene, exhibiting either an isolated vacancy or a substitutional nitrogen atom different kinds of images are to be expected, depending on the orbital character. (ii) Graphene/BN heterostructures absorb light over a broad frequency range, from the near-infrared to the ultraviolet region, exhibiting novel features induced by the stacking [3]. Peculiar features of their excitations are inter-layer excitons that can be modulated upon layer patterning. By choosing the stacking arrangement, the electronic coupling between the individual components can be tuned to enhance light-matter interaction. (iii) As demonstrated for azobenzene monolayers, graphene as a substrate strongly impacts the photo-switching behavior of molecules [4]. Despite the weak hybridization, the photo-absorption of the molecules is remarkably modulated. While substrate polarization reduces the band-gap of the adsorbate, enhanced dielectric screening weakens the attractive interaction between electrons and holes. Furthermore, excitations corresponding to intermolecular electron-hole pairs, which are dark in the isolated monolayers, are activated by the presence of the substrate. (iv) Finally, we ask how first- and second-order Raman spectra of graphene [5] are affected by strain that may be induced by an underlying substrate. References: [1] A. Gulans, et al., J. Phys.: Condens. Matter 26, 363202 (2014). [2] L. Pardini, S. Löffler, G. Biddau, R. Hambach, U. Kaiser, C. Draxl, and P. Schattschneider, Phys. Rev. Lett. 117, 036801 (2016). [3] W. Aggoune, C. Cocchi, D. Nabok, K.Rezouali, M. Belkhir, and C. Draxl, preprint. [4] Q. Fu, C. Cocchi, D. Nabok, A. Gulans, and C. Draxl, preprint. [5] A. Hertrich, C. Cocchi, P. Pavone, and C. Draxl, in preparation.

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