

Abstract Submitted
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Optical properties of hydrogenated graphene from first principles¹ SEBASTIAN PUTZ, MARTIN GMITRA, JAROSLAV FABIAN, University of Regensburg — We investigate the effect of hydrogen coverage on the optical properties of single-side hydrogenated graphene from first principles. To account for different degrees of uniform hydrogen coverage we calculate the complex dielectric function for graphene supercells of various size, each containing a single additional H atom. We use the Linearized Augmented Planewave (LAPW) method, as implemented in WIEN2k, to show that the hydrogen coverage strongly influences the complex dielectric function and thus the optical properties of hydrogenated graphene. The absorption coefficient in the visible range, for example, has different characteristic features depending on the hydrogen coverage. This opens up new possibilities of determining the hydrogen coverage of hydrogenated graphene samples in the experiment by contact-free optical absorption measurements.

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