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Single atom doping of graphene – A theoretical study

AMIR NATAN, Department of Physical Electronics, Tel-Aviv University, 69978 Tel-Aviv, Israel, TAMAR SEIDEMAN, Department of Chemistry, Northwestern University, Evanston IL 60208-3113, USA — We present first principles results and analysis for the electronic structure of chemically modified graphene. We show the relationship between different physical parameters and the electronic band structure of the modified material and its doping level. Finally, we discuss the possible effects of a substrate and of charge transfer patterns for device applications.

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