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**Graphene functionalization by single atoms doping - a theoretical study** AMIR NATAN[1], ELAD SEGEV, Department of Physical Electronics, Tel-Aviv University, Tel-Aviv, 69978, Israel, MARK HERSAM, Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208, USA, TAMAR SEIDEMAN, Departmen of Chemistry, Northwestern University, Evanston, IL 60208, USA — We present first principles results and analysis for the electronic structure of chemically modified graphene. We analyze the cases of fluorine adsorption and nitrogen substitution and show that a simple analytical model can describe the doping level as a function of dopant concentration for both cases. 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 substrate and of different dopant patterns on the band structure and possible applications.

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