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Edge Functionalization and Optical Excitations in Graphene Nanoflakes CATERINA COCCHI, S3 CNR-Nano, IT and University of Modena, IT, DEBORAH PREZZI, S3 CNR-Nano, IT, ALICE RUINI, S3 CNR-Nano, IT and University of Modena, IT, MARILIA J. CALDAS, University of Sao Paulo, BR, ELISA MOLINARI, S3 CNR-Nano, IT and University of Modena, IT — We investigate the effects of edge covalent functionalization on the opto-electronic properties of finite elongated graphene nano-flakes (GNFs). Following our previous work on nanojunctions[1], we compute mean-field ground state electronic properties and configuration-interaction UV-vis optical excitations at varying size and functionalization by means of semi-empirical methods. The character of the lowest energy excitations and the influence exerted on them both by length/width modulation and by the specific chemical properties of the terminating groups are analyzed in details. The role of local distortions spontaneously arising upon geometrical optimization is inspected. Nanoplasmonic-like features related to the spectrum of these elongated finite graphene nanostructures are also discussed. [1] C. Cocchi et al. J. Phys. Chem. Lett. 2, 1315 (2011)

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