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Concavity effects on the optical properties of aromatic hydrocarbons[1] MARILIA J. CALDAS, Institute of Physics, University of Sao Paulo, CATERINA COCCHI, DEBORAH PREZZI, Centro S3, CNR-Istituto Nanoscienze, Italy, ALICE RUINI, Centro S3, CNR-Istituto Nanoscienze, and Dept. of Physics, University of Modena and Reggio Emilia, Italy, ANNALISA FASOLINO, Institute for Molecules and Materials, Radboud University Nijmegen, The Netherlands, ELISA MOLINARI, Centro S3, CNR-Istituto Nanoscienze, and Dept. of Physics, University of Modena and Reggio Emilia, Italy — We address the modifications on the ground and excited state properties of polycyclic aromatic hydrocarbons (PAHs) induced by variations of concavity and π-connectivity. We study three series of PAHs, inspired by experimentally feasible systems, from hydrogen-saturated graphene flakes to concave "buckybowls" related to the formation of fullerene C_{60} and carbon nanotube caps. We work within the framework of Hartree-Fock-based semiempirical methods (AM1 and ZINDO/S), and our results are supported by a generally good agreement with the available data. We see clearly that the interplay between concavity and π-connectivity shifts the bright optical lines to higher energies, and introduces symmetry-forbidden dark excitations at low energy [1]. These features can be the basis for designing optical properties of novel curved aromatic molecules.

[1] C. Cocchi et al. submitted (2012).

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