Abstract Submitted for the MAR12 Meeting of The American Physical Society

Electronic structures of geometrically restricted nanocarbons ARTEM BASKIN, PETR KRAL, University of Illinois at Chicago — We use large scale ab-initio calculations to explore the electronic structures of graphene, graphene nanoribbons, and carbon nanotubes periodically perforated with nanopores. We disclose common features in electronic structures of these porous nanocarbons (PNCs) with nanopores of different size, shapes, and localization. We develop a unified picture that permits to analytically predict and systematically characterize metal-semiconductor transitions in PNCs, allowing mapping of their electronic structures on those in pristine nanocarbons [1]. In contrast to other studies, we show that porous graphene can be metallic for certain arrangements of the pores. When we replace pores by defects (such as SW 55-77), we observe similar features in the electronic structures of the formed nanocarbons. We also study magnetic ordering in these nanocarbons and show that the position of pores/defects can influence the ordering of localized electronic spin states. These periodically modified nanocarbons with highly tunable band structures have great potential applications in electronics and optics. [1] A.I. Baskin and P. Kral, Sci. Rep.1, 36 (2011).

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Date submitted: 09 Nov 2011

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