Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Structure, Stability, Edge States and Aromaticity of Graphene Ribbons TOBIAS WASSMANN, ARI PAAVO SEITSONEN, A. MARCO SAITTA, MICHELE LAZZERI, FRANCE MAURI, IMPMC, Paris, France — We determine the stability, the geometric, the electronic and magnetic structure of hydrogen-terminated graphene-nanoribbons edges as a function of the hydrogen content of the environment by means of density functional theory [1]. Antiferromagnetic zigzag ribbons are stable only at extremely-low ultra-vacuum pressures. Under more standard conditions, the most stable structures are the mono- and di-hydrogenated armchair edges and a zigzag edge reconstruction with one di- and two mono-hydrogenated sites. At high hydrogen-concentration "bulk" graphene is not stable and spontaneously breaks to form ribbons, in analogy to the spontaneous breaking of graphene into small-width nanoribbons observed experimentally in solution [2]. The stability and the existence of exotic edge electronic-states and/or magnetism is rationalized in terms of simple concepts from organic chemistry (Clar's rule). [1] T. Wassmann, et al. Phys. Rev. Lett. 101, 096402 (2008). [2] X. Li et al., Science 319, 1229 (2008); X. Wang et al., Phys. Rev. Lett. 100, 206803 (2008).

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Date submitted: 21 Nov 2008 Electronic form version 1.4