

Abstract Submitted
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Complex edge effects in graphene nanoribbons due to hydrogenation¹ BIPLAB SANYAL, Associate Professor, Uppsala University, Sweden, SUMANTA BHANDARY, Ph.D. student, Uppsala University, Sweden, MIKHAIL KATSNELSON, Professor, Radboud University Nijmegen, The Netherlands, OLLE ERIKSSON, Professor, Uppsala University, Sweden — We have performed density-functional calculations as well as employed a tight-binding theory, to study the effect of hydrogenation of zigzag graphene nanoribbons (ZGNR). We show that each edge C atom bonded with 2 H atoms open up a gap and magnetism collapses for small widths of the nanoribbon. However, a re-entrant magnetism accompanied by a metallic electronic structure is observed from eight rows and thicker nanoribbons. The electronic structure and magnetic state are quite complex for this type of termination, with sp^3 bonded edge atoms being nonmagnetic whereas the nearest neighboring atoms are metallic and magnetic. We have also evaluated the phase stability of several thicknesses of ZGNR and demonstrate that sp^3 bonded edge atoms with 2 H atoms at the edge can be stabilized over 1 H atom terminated edge at high temperatures and pressures.

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