Topological defect clustering and plastic deformation mechanisms in functionalized graphene

RICARDO NUNES, JOICE ARAUJO, HELIO CHACHAM, UFMG-Brazil — We present ab initio results suggesting that strain plays a central role in the clustering of topological defects in strained and functionalized graphene models. We apply strain onto the topological-defect graphene networks from our previous work [1], and obtain topological-defect clustering patterns which are in excellent agreement with recent observations in samples of reduced graphene oxide [2]. In our models, the graphene layer, containing an initial concentration of isolated topological defects, is covered by hydrogen or hydroxyl groups. Our results also suggest a rich variety of plastic deformation mechanism in functionalized graphene systems.


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