From multi-layered graphene to diamond film of nanometer thickness. Chemically induced phase transformation

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The dominant contribution of the graphene surface allows to modify its structure by surface functionalization processes such as hydrogenation, oxidation, fluorination, etc. A transformation of sp^2-hybridized graphene to sp^3-hybridized diamond film (diamane [1]) cannot be described by the bulk diamond-graphite phase diagram and requires to take into account graphene surface contribution. For instance, a nanoscale transformation of functionalized graphene to diamane (i.e. chemically induced phase transition) was developed in our previous work under conditions of full and uniform functionalization of graphene surface [2]. Despite of the successful experimental realization of prediction a lot of questions remain unanswered like "why formation of diamond nanofilm was observed only for the case of bilayer films?", "what the mechanism of phase transition from graphene to diamane?", "what the final structure of the resulted diamond film and how it depends on the external conditions?". All of them require extension of the somewhere oversimplified theory and take into account a new phase nucleation process, describe the "reaction path" and nucleation barrier. We answered for these questions by carrying out *ab initio* computation which allows to directly observe a nanoscale diamondization process and estimate a nucleation barrier. We show that diamond formation considerably depends on graphene layers number, their packing, type and arrangement of adatoms as well as external parameters and therefore requires they fine tuning in the further experiments [3].

References

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