Abstract Submitted
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Ab initio study of single and double vacancies in graphene[1] MAHMOUD HAMMOURI, IGOR VASILIEV, New Mexico State University — Graphene is a promising material for semiconductor engineering and other applications. The introduction of point defects such as vacancies can make graphene a magnetic material. We calculate the density of states and the band structure of a single and double vacancy in a graphene using periodic supercell containing 64, 72, and 128 carbon atoms. Our calculations are performed using the SIESTA density functional electronic structure code combined with the generalized gradient approximation for the exchange correlation functional.

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