

#21 Topic: A computational model of graphene

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Abstract:

Graphene is a very interesting material for a theoretical study. Among its many properties, it is a 2D crystal (i.e. it tends to form a single sheet one atom thick) in its purest form but defects will generate a buckling in the material. We introduce a computational model of buckled graphene, present some preliminary results obtained from it and discuss the main challenges of the model.