

## STUDY OF STRUCTURED GRAIN BOUNDARIES IN GRAPHENE USING A TIGHT BINDING BASED MODEL

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**Key words:** *Graphene, Tight binding, Grain boundaries, Thermal stability.*

In the field of electronics, due to its excellent mechanical and electrical properties, graphene has become the most promising material for the production of next generation thin and flexible graphene-based electronic components. Pristine defect-free graphene has no band-gap and is of limited use for semiconductor-based electronics. It was found experimentally that the Stone-Wales defects could change the local density of states, however, is not expected to introduce band gaps. Therefore, many attempts have been made to engineer band gaps in graphene. Among other mechanisms, it has been shown theoretically that grain boundaries might insert band gaps. In order to identify appropriate geometrical configurations, we have carried out an appraisal of the stability and dynamics of grain boundaries in graphene for different misorientation angles at finite temperature and up to extremely high temperatures. To this end, we have developed a simulation tool based on lattice harmonics and tight-binding potentials.