25e Congrès Général de la Société Française de Physique

ID de Contribution: **182** Type: **Poster**

Molecular dynamics' simulations of carbon structure with LAMMPS

The first part of this work focuses on finding a potential to describe graphitic materials with their registry dependance. Five different potential have been studied by checking the C-C bond-lengh in Graphene, the interlayer distance in Graphite, the binding energy shift for different stacking configuration and the diametre at which collapsed carbon nanotubes (CCNT) are more stable than carbon nanotubes. The second part is about studying chiral CCNT's self-twisting through thermal treatment simulation in a NVT environment with a focus on the registry's implication.

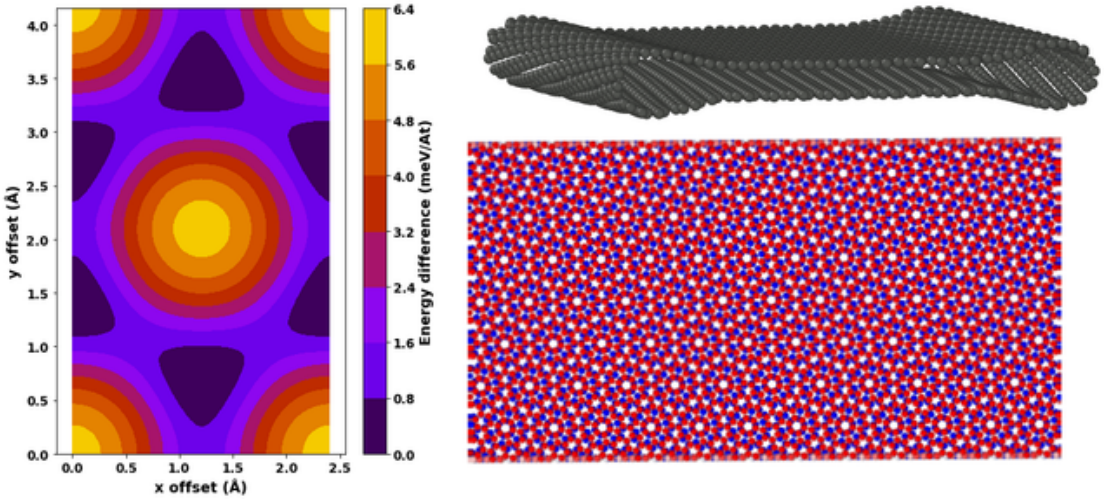

Figure 1: Graphite binding energy registry dependance (left), Chiral CCNT (up right),Moiré pattern on a Chiral CCNT (down right)

Choix de session parallèle

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Classification de Session: Séance Poster