Contribution ID: **64** Type: **Poster Presentation**

Structural stability of some graphene oxide formations

Thursday, 11 July 2019 15:00 (2 hours)

The classical molecular dynamics was used to study various forms of graphene oxide possible formations focusing mainly on the structural stability. The structures were modelled at 300 K through the NVT Evans ensemble. Variations of the total energy against the a-axis was explored in which the equilibrium properties were computed. Pair distribution functions as well as structure factors were plotted. In the plots nearest neighbour distances and their neighbouring number of atoms were obtained. To probe the mobility of oxygen in the systems, the mean square displacements as well as the velocity auto-correlations were plotted.

Apply to be
 considered for a student
   award (Yes / No)?

Yes

Level for award
 (Hons, MSc,
   PhD, N/A)?

MSc

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Session Classification: Poster Session 2

Track Classification: Track G - Theoretical and Computational Physics