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Structural Stability of Graphene Oxide

The structural properties of graphene oxide (GO) were studied through the classical molecular dynamic simulations. The variation of energy and temperature for the NVT, NPT and NVE ensemble was explored, and in the process the entropy was computed to determine the degree of disorder in the system. The pair distribution functions were plotted for carbon-carbon atoms and the nearest neighbouring distance and their neighbouring atoms were obtained. Furthermore, the structure of GO was simulated at various temperatures for NVT and NPT ensemble and the difference in the structures was discussed.

Presenter Biography

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