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# Stability of edge oxidized graphene nanoribbons

Graphene has been keeping a premier position in nanoscale sciences and technologies in this decade, because of their unique geometric and electronic structures, allowing them an emerging material for functional devices in the near future. To utilize graphene for the devices, it is mandatory to control their geometries and to elucidate their stability against the formation of hybrid structures with foreign materials. Edge stability against chemical attachment is one of important factors to determine the graphene geometries. In this work, we aim to elucidate the energetics of GNRs by the edge oxidization in terms of their detailed edge geometries, using the density functional theory with generalized gradient approximation. As for the structural model, we consider five GNRs with edge angles from 0° (armchair edge) to 30° (zigzag edge) (Fig.1).

Figure 2 shows the adsorption energy of O atom to clean edges of GNRs with edge angles from 0° to 30°. The adsorption energy strongly depends not only on the edge angle but also on the adsorbing atomic site in each edge shape. Our calculations demonstrate that the edges with the zigzag shape are preferentially oxidized compared with the edge with the armchair shape. Furthermore, O atom attached to the step edge lead to the substantial structural deformation around the edges. By performing the finite temperature molecular dynamics (MD) simulations, we found that several metastable structures undergo the structural transition into more stable structures at the elevated temperature (Fig.3).

## Figures

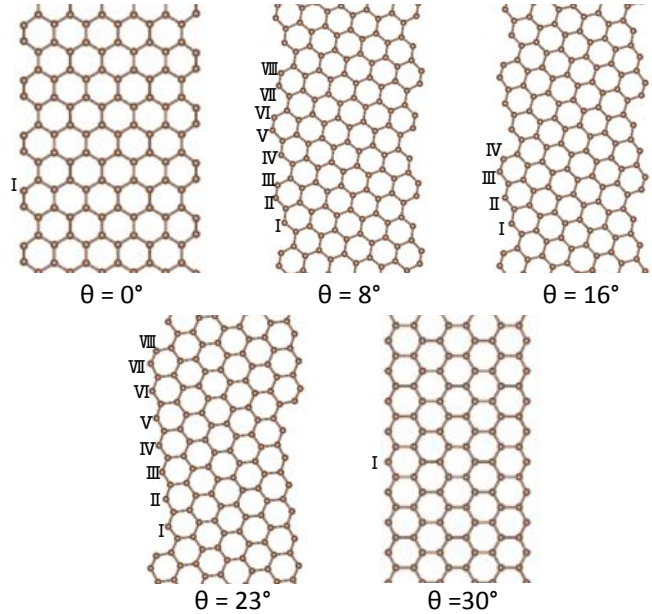


Fig.1 Optimized structures of GNRs with clean edges.

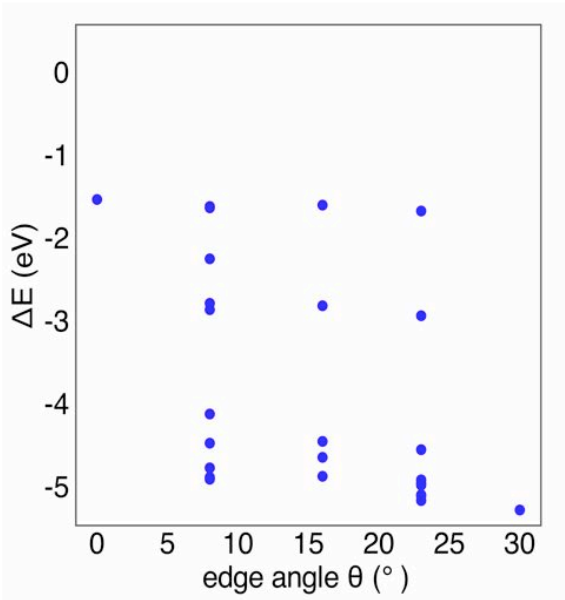


Fig.2 Adsorption energy of oxygen to GNRs.

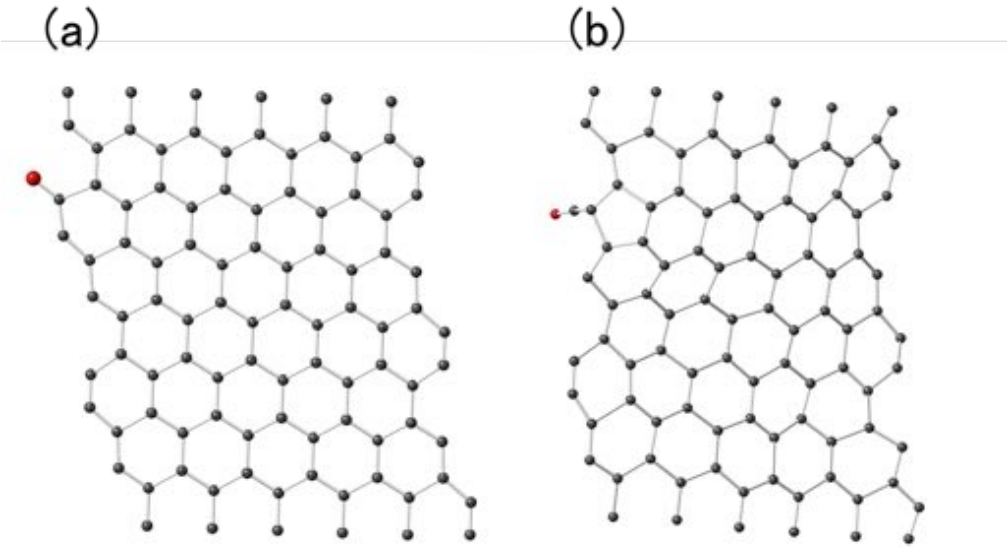


Fig.3 Snap shots of (a) a metastable oxidized structure and (b) a reconstructed structure after the finite temperature MD calculation.