# Simulations of the Reduction of Graphene Oxide Suspensions by Hydrazine

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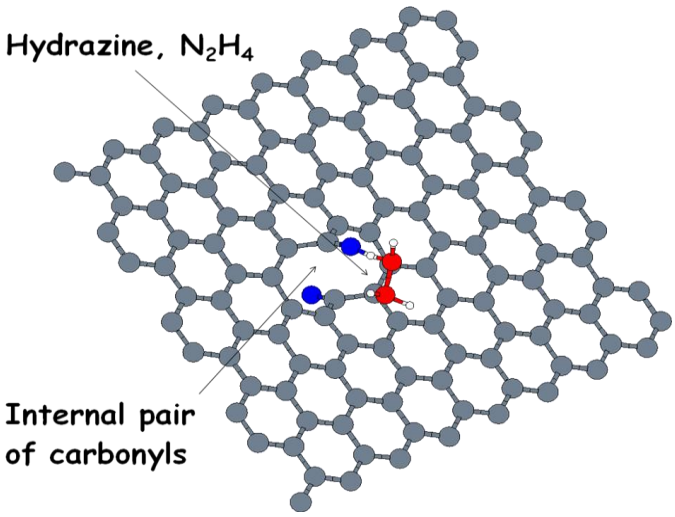
Simulations of the interaction of hydrazine with graphene oxide have been carried out to understand recent experiments of the reduction of graphene oxide by hydrazine [1]. According to chemical analysis, hydrazine-reduced graphene oxide still contains a certain amount of oxygen functionalities that cannot be removed. Even in the most reduced materials the O/C atomic ratio, 0.08, indicates the presence of a significant amount of residual oxygen. Previous reports on graphene oxide reduction by hydrazine also support the idea that chemical reduction has an intrinsic limit, which is not well understood. A possible explanation of the residual oxygen is the presence of oxygen functionalities in graphene oxide, before the reduction processes, that can not be removed by hydrazine.

We have done DFT calculations of the interaction of hydrazine with several isolated oxygen functionalities on a graphene layer, namely epoxy and hydroxyl groups and a carbonyl pair inside a graphene layer. The results of the calculations indicate that hydrazine could reduce the epoxy groups to hydroxyls and the hydroxyl groups can be reduced to water, which is eliminated from the graphene. In contrast, hydrazine is not able to reduce the carbonyls to form C-O-H groups. We have also done DFT calculations of the interaction of hydrazine with epoxy and hydroxyl groups on a coronene. The results on the coronene differ from those on graphene. This indicates that a finite portion of graphene, the coronene, is not a good model to represent the whole graphene oxide layer, and therefore results on coronenes have to be taken with caution. In summary, our results indicate that a pair of neighbour carbonyls could explain the residual oxygen found experimentally in reduced graphene oxide.

## References

[1] M. J. Fernández-Merino, L. Guardia, J. I. Paredes, S. Villar-Rodil, P. Solís-Fernández, A. Martínez-Alonso, and J. M. D. Tascón, J. Phys. Chem. C 114, (2010) 6426–6432

## Figures




*Hydrazine interacting with an internal pair of carbonyls on graphene*