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The Surfaces of Nanodiamonds: A Modeling Perspective

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Nanodiamonds (NDs) are carbon-based nanoparticles that have attracted significant attention due to the possible applications in a wide range of fields – from nanocomposites and tribology to quantum sensing and nanomedicine [1]. This can be attributed to their specific optical, mechanical, and chemical properties among which the versatile surface chemistry has proven to be particularly beneficial in the biomedical area [2].

In general, the surface features are the most critical factors regarding the applications of NDs [3]. Even if the cores of NDs play an important role, the interactions between them and surrounding environment are mediated by the interface at the surface, therefore the behavior of NDs in a medium is still dependent on the surface chemistry. By controlling the functional groups that NDs possess, properties such as colloidal stability, hydrophilicity, and reactivity can be tuned for the desired applications [4]. The surfaces of NDs can be covered with a variety of functional groups by applying, for example, hydrogenation, hydroxylation, amination or carboxylation procedures (see Fig. 1) [5].

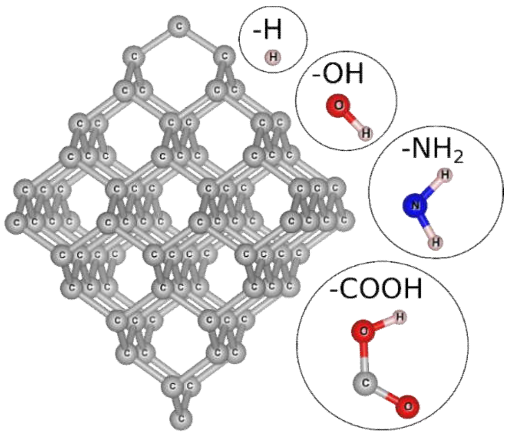

Fig. 1. Nanodiamond and its possible surface functionalization schemes.

The main aim of this work is to model NDs the surfaces of which would be fully grafted with the aforementioned functional groups. We seek to find out the optimal surface structure which would be consistent with the experimental findings and thereby could be used for the further theoretical investigation for the properties of interest. The performed quantum chemistry calculations reveal that, compared to the others, the carboxylic acid groups are harder to deal with pointing to the need for the more sophisticated modeling strategy.

References

1. S. L. Y. Chang, P. Reineck, A. Krueger, V. N. Mochalin, ACS Nano, **16** (2022) 8513.
2. D. H. Jariwala, D. Patel, S. Wairkar, Mat. Sci. Eng. C, **113** (2020) 110996.
3. N. Nunn, M. Torelli, G. McGuire, O. Shenderova, Curr. Opin. Solid State Mater. Sci., **21** (2017) 1.
4. M. B. A. Olia, P. S. Donnelly, L. C. L. Hollenberg, P. Mulvaney, D. A. Simpson, ACS Appl. Nano Mater., **4** (2021) 9985.
5. A. Krueger, D. Lang, Adv. Funct. Mater., **22** (2012) 890.