Computational study on the electronic *g*-tensors of nanodiamonds

Šarūnas Masys, Jelena Tamulienė

Institute of Theoretical Physics and Astronomy, Vilnius University, Saulėtekio Avenue 3, LT-10257 Vilnius, Lithuania

E-mail: sarunas.masys@tfai.vu.lt

Nanodiamonds (NDs) belong to a family of carbon-based nanomaterials that recently gained a lot of attention in such biomedical areas as tissue engineering, labelling, quantum sensing, and drug delivery. Concerning the latter, a combination with the bioimaging capabilities could make NDs a very promising platform for the clinical theranostic applications, thereby allowing a more effective exploitation of these nanoparticles.

In order to fully utilize the bioimaging potential of NDs using such techniques as magnetic resonance imaging based on Overhauser effect (OMRI), which in turn requires a paramagnetic reservoir to be present in the system, one has to be aware of their magnetic properties. In this work, density functional theory calculations were carried out seeking to find out the influence of the shape, size, and surface functionalization of NDs on their electronic *g*-tensor values. Substitutional nitrogen atoms and dangling bonds at the surface – the most common paramagnetic defects observed in NDs – were considered as a paramagnetic reservoir needed for OMRI and therefore introduced into NDs of octahedral, tetrahedral, and cubic shape. Regarding the surface functionalization schemes, hydrogenation together with fluorination and chlorination were chosen. The obtained results can be highly useful for the experimental studies of NDs, since they can help to analyze and interpret complicated electron paramagnetic resonance spectra.