Probing the interaction of DNA nucleobases with diamondoids through atomistic simulations

Ganesh Sivaraman
Institute for Computational Physics, Universität Stuttgart, 70569 Stuttgart

Maria Fyta
Institute for Computational Physics, Universität Stuttgart, 70569 Stuttgart

Understanding the interaction of biomolecules with materials is essential in view of the variety of potential applications in the integration of these two systems can lead to. To this end, we investigate the interaction of DNA with diamondoids. The latter are a wide family of tiny hydrogen- terminated diamond clusters which have shown high technological potential ([1],[2]). We probe this interaction through quantum-mechanical computer simulations. We focus on the hydrogen bonding possibilities of the different DNA nucleobases with the lower diamondoids with respect to their relative distance and orientation ([3],[4]). Our aim is also to investigate ways to promote the binding between these two units. Accordingly, we functionalize the diamondoid by replacing one of it's hydrogens with atomic groups, such as amine groups, and study the respective binding probabilities of these two molecules. We probe this binding through the binding energy and the electronic structure of the nucleobase-diamondoid system and reveal the specific role of their frontier orbitals. In the end, we discuss the importance of our results in view of realizing a diamondoid functionalized nanopore for electrically reading out the DNA sequences ([5]).

[1] Xue, Y.; Mansoori, G.A.,Int. Jou. Nanosci **7**, (2008): 63

[2] Xue, Y.; Mansoori, G.A.. Int. J. Mol. Sci.**11** (2010): 288

[3] Joel Ireta, Jörg Neugebauer and matthias Scheffler, J. Phys. Chem. A **108** (2004):5692

[4] Burns et al. J. Chem. Phys. **134** (2011):084107

[5] He, Haiying et al. J. Phys. Chem. C, **112** (2008):3456