

Modified diamondoids for sensing applications

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Diamondoids are tiny diamond-like cages which are hydrogen terminated and can occur in various sizes and with a diverse type of modifications giving rise to novel biotechnological applications [1, 2, 3]. In this work, based on quantum-mechanical calculations we study the effect of doping and functionalization of diamondoids on their structural characteristics and electronic properties [4]. For this, we use different dopants and atomic groups and focus on the band-gap variations and the influence of the molecular orbitals in the case of the lower diamondoids, adamantane up to heptamantane (Fig. 1(a)). At a second step, we turn to the functionalized diamondoids and use these as probes to sense DNA molecules. Modified diamondoids can form hydrogen bonded complexes to DNA nucleobases tuning their electronic properties [5] (Fig. 1(b)). Accordingly, we have observed that these small modified diamond-like cages are able to distinguish between small and large DNA nucleobases based on a difference up to 1 eV in the electronic band-gaps of the respective complexes [6]. In the end, we discuss the possibility to sequence DNA through diamondoid-functionalized nanopores using quantum transport measurements.

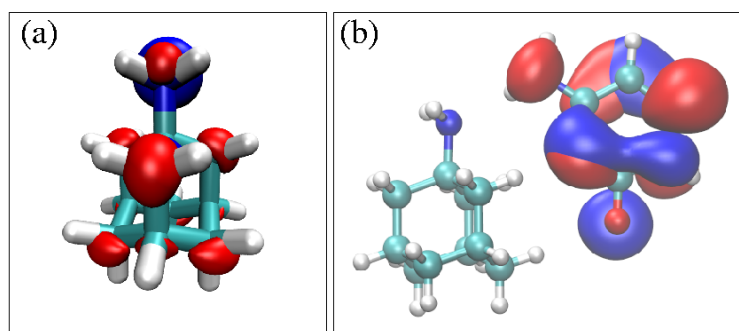


Figure 1: (a) A NH_2 -modified diamondoid. (b) The same diamondoid is probing a DNA nucleobase. The frontier (highest occupied in blue and lowest unoccupied in red) molecular orbitals are shown in both panels.

References

- [1] J. E. Dahl, S. G. Liu, and R. M. K. Carlson, *Science* **299**, 96 (2003).
- [2] W.L. Yang *et al*, *Science*, **316**, 1460 (2007).
- [3] H. Schwertfeger, A. A. Fokin, and P. R. Schreiner, *Angew. Chem. Int. Ed.* **47**, 1022-1036 (2008).
- [4] B. Adhikari and M. Fyta, under review (2014).
- [5] G. Sivaraman and M. Fyta, *Nanoscale* **6**, 4225 (2014).
- [6] F.C. Maier and M. Fyta, under review (2014).

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