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Modeling of M-DNA Using Dispersion-Augmented Density Functional Tight Binding: Benchmarks with RI-MP2 and CCSD(T) as Reference

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We present quantum chemical studies in the attempt to use biological systems as building blocks for a new breed of “biochemistry-inspired” molecular computer components, such as the case of M-DNA recently presented by Tanaka et al.¹ Here, the electronic structure associated with the chain of Cu²⁺ ions inside the double helix is dependent on the type of nucleobase pairs they are attached to, and therefore one has to explicitly take into account all base pairs at the quantum chemical level, while possibly leaving the phosphate and sugar backbone for a low-level MM treatment in a hybrid approach such as ONIOM. The problem with a quantum chemically modeling the DNA bases is, however, that conventional single-determinant wavefunction-based methods such as density functional theory is not capable to account for the effects of π -stacking due to the lack of dispersion interaction in their formalisms. As a first step towards quantum chemically modeling conductance through DNA-based computer devices we have performed benchmark calculations at the density functional tight binding plus dispersion (DFTB-D), resolution-of-identity MP2 (RI-MP2), and CCSD(T) levels of theory on dimers, trimers, and higher oligomers of Zn-metalized DNA base pairs with explicit consideration of the DNA backbone.

¹K. Tanaka *et al.* Nature Nanotechnol. **1**, 190 (2006)