[L7] Ab Initio Calculation of Polymononucleotide, a Model of B-type DNA

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The electronic structure calculations of the polymononucleotides as a B-type model-DNA, (poly-(guanine) poly-(cytosine)) and (poly-(adenine) poly-(thimine)) double helixes including sodium phosphate, hereafter referred as (poly-dG poly- dC) and (poly-dA poly-dT), double helix model polymer is performed by means of *ab initio* crystal orbital method adapting the screw axis-symmetry[1-2] which results in great reduction of computational efforts. The calculations are also performed for polymers with and without the sodium phosphate and without the sodium phosphate and the sugar, which is just the polymer of the base pair, for a comparison. Energy band structures are calculated at 6-31G level.

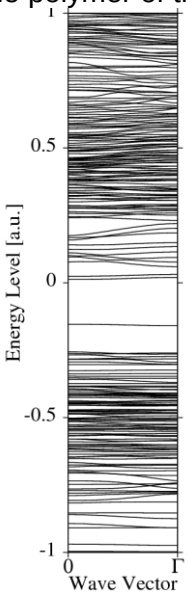

Fig.1 The energy band structure of (poly-dG poly-dC).

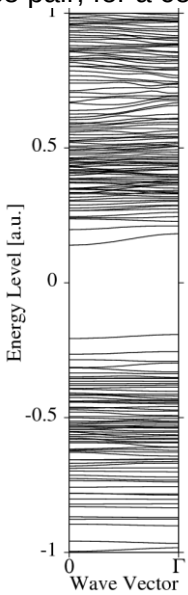

Fig.2 The energy band structure of (poly-dG poly-dC) without sodium phosphate.

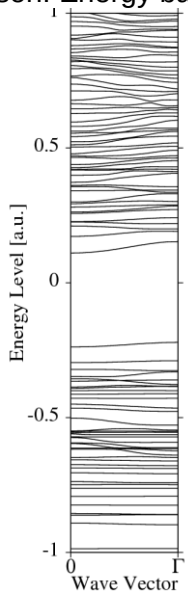

Fig.3 The energy band structure of (poly-dG poly-dC) without sodium phosphate and sugar.

Figure 1 shows the energy band structure of (poly-dG poly-dC). Figure 2 shows that of (poly-dG poly-dC) without sodium phosphate and Figure 3 shows that of (poly-dG poly-dC) without sodium phosphate and sugar.

These figures shows that the inclusion of the sodium phosphate is necessary to describe the electronic structures of DNAs. We also made the same calculations on the (poly-dA poly-dT) polymer and the results were similar.

In addition, we also calculated (poly-dG), (poly-dC), (poly-dA), and (poly-dT) single helixes to see the effects of the hydrogen bonds between the base pairs on the energy band structures.

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Bibliography:

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