Nucleic acid bases and analogues: electronic structure with LCAO.

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We study the electronic structure of nucleic acid bases and analogues with the linear combination of atomic orbitals (LCAO) method taking only p_z atomic orbitals into account, in other words using a type of Hückel model but with the parametrization proposed by Hawke *et al.* [1]. This parametrization can be employed to molecules containing carbon, nitrogen, or oxygen atoms with sp^2 hybridization. For the diagonal matrix elements of the LCAO description, four empirical parameters are used, corresponding to carbon, nitrogen with one or two p_z electrons and oxygen atoms. For the non-diagonal matrix elements between neighbouring atoms the bond-length dependent formula of Harrison is used [3]. The method has already been successfully applied among other molecules to adenine, guanine, cytosine, thymine, and uracil [1] and subsequently used to obtain the tight binding parameters pertinent to charge transfer along DNA [2]. Here we apply it to nucleic acid bases and analogues e.g. purine, 1,4-dioxide pyrazine, 1H-imidazole, 1H-indazole, 1H-benzimidazole, pyrazine, pyrimidine, and so on. We compare our results to experimental ionization energies and HOMO-LUMO gaps.

References

[1] L.G.D. Hawke, G. Kalosakas, C. Simserides, Molecular Physics 107 (2009) 1755.

[2] L.G.D. Hawke, G. Kalosakas, C. Simserides, Eur. Phys. J. E 32 (2010) 291; ibid. 34 (2011) 118.

[3] W.A. Harrison, *Electronic Structure and the Properties of Solids*, 2nd ed. (Dover, New York, 1989); *Elementary Electronic Structure* (World Scientific, River Edge, NJ, 1999).

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