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Electronic structure of purines, pyrimidines and similar molecules with LCAO

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Abstract: We study the electronic structure, including the lowest ionisation and excitation energies, and the transition dipole moments of biologically important heterocyclic planar molecules like purines, pyrimidines and similar molecules e.g. carbazole, luminol, acetophenone, phenanthroline etc. We use the linear combination of atomic orbitals (LCAO) method, taking only p_z atomic orbitals into account. In other words, we use a type of Hückel model but with the parametrizations proposed either by Hawke *et al.* [1] or by Mantela *et al.* [2]. These parametrizations can be employed to molecules containing carbon, nitrogen, or oxygen atoms with sp^2 hybridization. For the diagonal matrix elements, 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, bond-length dependent formulae like the one of Harrison [3] are used. The methods have already been successfully applied among other molecules to adenine, guanine, cytosine, thymine, and uracil [1,2] and used to obtain the tight binding parameters pertinent to charge transfer along DNA [4]. We compare our results to experimental ionization energies, HOMO-LUMO gaps and transition dipole moments.

[1] L.G.D. Hawke, G. Kalosakas, C. Simserides, Molecular Physics 107 (2009) 1755
[2] M. Mantela, A. Morphis, M. Tassi and C. Simserides, Molecular Physics 114 (2016) 709
[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)
[4] L.G.D. Hawke, G. Kalosakas, C. Simserides, Eur. Phys. J. E 32 (2010) 291; ibid. 34 (2011) 118