CALCULATION OF NMR CHEMICAL SHIFTS USING A DENSITY-FUNCTIONAL BASED TIGHT-BINDING SCHEME - APPLICATION TO FULLERENE DERIVATIVES

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The IGLO-DFTB method [1], which is the use of the IGLO technique on Density-Functional based non-orthogonal Tight-Binding (DFTB) molecular orbitals, is presented. The method is illustrated by test calculations on silanes and its application to fullerene derivatives such as the C_{60} dimer [1], C_{119} [2] and the endohedral fullerene Sc_3NC_{68} [3].

[1] T. Heine, G. Seifert, P.W. Fowler, and F. Zerbetto, *J. Phys. Chem. A* 103 (1999) 8738.

[2] T. Heine, F. Zerbetto, G. Seifert, and P.W. Fowler, *J. Phys. Chem. A* 104 (2000) 3865.

[3] S. Stevenson, P.W. Fowler, T. Heine, J.C. Duchamp, G. Rice, T. Glass, K. Harich, E. Hajdu, R. Bible, H.C. Dorn, *Nature* 408 (2000) 427.