A Quantum Leap Into the Future of Chemistry

What's New in Q-Chem

Feature 9

Hirshfeld Atomic Populations

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$$q_A = Z_A - \int dr \frac{\rho_A^0(r)}{\sum_B \rho_B^0(r)} \rho(r)$$

Hirshfeld atomic populations are an alternative definition of atomic charges to the standard Mulliken and Lowdin schemes, and they provide a clear partitioning of the electron density. We have implemented the calculation of Hirshfeld charges into Q-Chem as a post-SCF step. Hirshfeld's scheme can be shown to yield an optimal partitioning of atomic densities in an information theoretic sense, and it can be useful to compare the results of Mulliken populations with other methods. Hirshfeld populations can be calculated at the end of any molecular calculation.

The illustration shows the Hartree-Fock atomic populations of a few small organic molecules are tabulated with Mulliken and Hirshfeld atomic populations. The charge on each carbon atom is shown. Note that the magnitude of the Hirshfeld charges is in general smaller than for Mulliken, and the Hirshfeld charges are also less basis-set dependent, as expected for a density-based population scheme.

Molecule	Method	3-21G	6-31G	6-31G*
C_2H_2	Mulliken	-0.33	-0.32	-0.28
	Hirshfeld	-0.10	-0.10	-0.10
CH_4	Mulliken	-0.79	-0.62	-0.66
	Hirshfeld	-0.09	-0.11	-0.10
CO	Mulliken	0.43	0.33	0.27
	Hirshfeld	0.11	0.13	0.13

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For more information on how to use this feature, refer to the Q-Chem Manual, Section ____

For more new features, visit: www.q-chem.com/whatsNew4.html

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