A new variational, information theory based atoms in molecules method

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A new iterative Hirshfeld [1,2] type AIM method, called Hirshfeld-I-Lambda, is presented. The weight function that defines the AIM is constructed by minimizing the information loss on formation of the molecule, with explicitly requiring that the promolecular densities integrate to the same number of electrons as the AIM densities constructed. The atoms defined by this AIM method are the ones that minimize the information lost upon formation of the molecule out of its isolated atoms. [3-7] The resulting Hirshfeld-I-Lambda AIM scheme is examined and discussed.

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