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Title: A computational probe for the study of molecular electric fields

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Abstract: We propose the use of a fictitious isotopic probe, similar to the HD molecule, to investigate molecular environments, independently of the accurate representation of the electronic density and its gradient. HD has a small dipole moment due to its mass asymmetry. We explore the possibility of handling the finite nuclear masses with our code ISOTOPE [1, 2] in electronic calculations, to introduce a fictitious probe with a large and a small nuclear mass, and freeze the "internuclear" distance, so to create an appropriate the dipole probe.

As the probe interacts with a molecule, we subtract the Born-Oppenheimer energy from the total energy, so that the interaction energy is reduced to two classical terms: the interaction of the dipole moment with the molecular electric field and the polarization of the molecule by the dipole, the second being usually much smaller than the first. These two energy terms can be isolated either by rotating the dipole or by their behaviour with the distance.

The probe can evaluate, for example, the vector electric field created by a molecule in specific points. For this we just flip the dipole from its position of least energy (field direction), calculate the energy difference, and divide it by the dipole moment (field strength). Applications will be presented for H_2, H_2O clusters and other systems.

Key-words: Molecular electric field, isotopic probe
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References:

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