11th International Conference
on Advanced Materials
Rio de Janeiro Brazil
September 20 - 25
ICAM2009

DFT calculations of isotopic (including Ps) effects in water clusters

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Abstract – We explore further an upgrade of the DFT – DeMon2k package to study effects on the electronic level of replacement of H atoms with D (deuterium) atoms. We also consider positronium Ps (e^+e^-) a light isotope of H and perform exploratory calculations with the resulting exotic clusters.

The performance of an upgrade of the DeMon2k [1] to include finite nuclear mass effects on both the potential energy surfaces and electronic wavefunction [2] has been discussed in the last ICAM. Now we perform applications to study the effects isotopic substitution of H atoms in water clusters $(H_2O)_n$, n=2,3,4,5,6,8. Changes in minimum energies and geometries, symmetry breaking and resulting isotopic electrical dipole moments as well as on the hydrogen bonds are reported.

We then consider the possibility of having a water cluster with replacement of one of the H atoms with a Ps (e^+e^-) exotic atom and discuss how a system like this could be produced and observed.

Suported by Fapemig and CNPq.

References

1. A. M. Koster et al, *Experimental Version of DeMon2k, 2006.*
2. J. R. Mohallem et al, J. Phys. Chem. A **112** (2008) 8896.