Quantum models of confined hydrogen species.

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Abstract: Hydrogen species like H_2, H and H_2^+ confined by nanoscopic potential wells are getting much interest. Their properties can be revealed by full *ab initio* simulation based on Quantum Diffusion Monte Carlo (QDMC) methods.

There has been great interest in recent years in quantum computation of the properties of small species based on hydrogen nuclei and electrons, both atomic and molecular, such as H, H_2^+, H_2, and which are confined by a potential well [1]. The reasons for this interest, which can be traced back to Schrodinger, are linked to the possibility of describing species of interest for astrophysics under high pressure conditions and species of interest for solid state physics inside crystals defects or molecular cages. The reason for the intense recent research activity is that very direct *ab initio* methods exploiting the possibilities offered by modern computing systems allow one to study a great variety of systems. And in fact, this variety is much greater than it appears at first glance, since hydrogen-based species include neutral species, positive and negative ions, monoatomic, diatomic, and even triatomic species such as H_3^+. Potential wells of potential interest for applications have spherical, cubic, polyhedral, and spheroidal shapes.

Our research group in this field has been operating for several years, but the activity has had a great acceleration in the PNRR context. Our trademark is the systematic use of the Quantum Diffusion Monte Carlo method (QDMC) [2] which allows, thanks to the development of native programs, to study any combination of system and shape for the cavity with minimal adaptations of the code.

In this way we were among the first to study the excited repulsive molecular states to show that they behave in a similar way to the bound ones under high pressure conditions [3]. We were also the first to study these systems with potential wells notoriously difficult to treat in the context of quantum mechanics, octahedral and even icosahedral ones [4]. We studied the ionization and dissociation due to a static field of these confined species and their polarizability [5,6]. Some of the results obtained are quite surprising

References

[1] Sen, K. D., & Sen, K. D. (Eds.). (2014). *Electronic structure of quantum confined atoms and molecules*, Springer.
[2] Micca Longo, G., Coppola, C. M., Giordano, D., & Longo, S. (2021). *The unbiased diffusion Monte Carlo: a versatile tool for two-electron systems confined in different geometries.* The European Physical Journal D, 75, 1-7.
[3] Micca Longo, G., Longo, S., & Giordano, D. (2015). *Spherically confined H2+: Σg+ and Σu+ states.* Physica Scripta, 90(2), 025403.
[4] Longo, S., Lonigro, D., Lerario, G., Stripoli, C., & Micca Longo, G. (2023). *Quantum states of H2+ and H2 in an icosahedral potential well.* The European Physical Journal D, 77(2), 29.
[5] Micca Longo, G., & Longo, S. (2024). *Electric field induced dissociation of a confined hydrogen molecule.* Chemical Physics Letters, 856, 141643.
[6] Micca Longo, G., & Longo, S. (2024). *Diffusion Monte Carlo calculations of the polarizability of a confined hydrogen atom: benchmarking and application to high symmetry wells*. Physica Scripta, 99(2), 025409.