Electrons as an environment for nuclei within molecules: a quantitative assessment of their contribution to a classical-like molecular structure

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ABSTRACT

Molecular structure is often considered as emerging from the decoherence effect of the environment. Electrons are part of the environment of the nuclei in a molecule. In this work, their contribution to the classical-like geometrical relationships often observed between nuclei in molecular systems is investigated. Reduced density matrix (RDM) elements are evaluated from electron-nucleus wave functions. The computational results show that the electrons play a role in the localization of the nuclei around specific geometries. Although the electronic environment alone cannot explain molecular symmetry-broken isomers, it can contribute to their dynamical stability by reducing off-diagonal RDM elements.

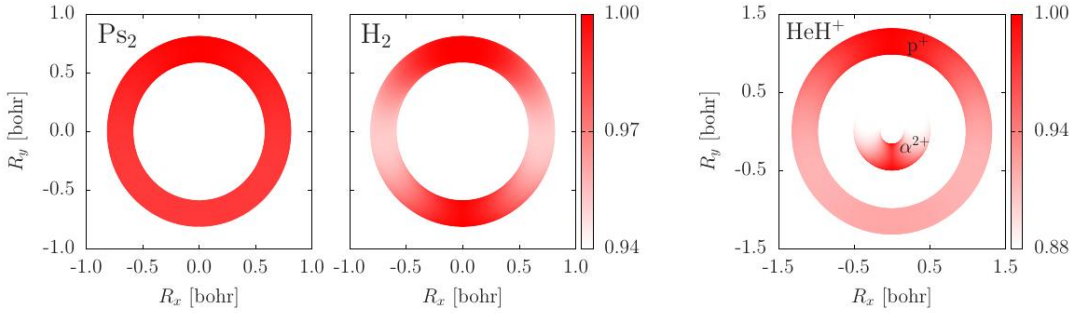

FIG. 6: Orientational (de)coherence measured by the suppression of the off-diagonal nuclear density with respect to the diagonal elements, $\rho_{0,n}(R, \hat{O}_\vartheta R)/\rho_{0,n}(R, R)$. The figure shows the xy cut of the three-dimensional function (the width of the shells is arbitrarily chosen to visualize the change of the off-diagonal normalized density with the angle). The upward (downward) vertical direction correspond to zero rotation angle ϑ for the positron and the proton (α-particle).

References

[1] Patrick Cassam-Chenaï, Edit Mátyus, Electrons as an environment for nuclei within molecules: a quantitative assessment of their contribution to a classical-like molecular structure, hal-02948537

[2] Edit Matyus, Patrick Cassam-Chenai, Orientational decoherence within molecules and emergence of the molecular shape, arXiv:2011.02810