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"Interactions in oxygen: from the gas to high pressure solid phases"

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Molecular oxygen in its ground electronic state, $O_2(^3\Sigma^-_g)$, is a open-shell magnetic system and an improved knowledge of the intermolecular interactions will have implications in the understanding of the substance in all its phases. We have recently obtained a global *ab initio* Potential Energy Surface (PES) **[1]** for the dimer, $O_2(^3\Sigma^-_g)$+$O_2(^3\Sigma^-_g)$, based on RCCSD(T) calculations for the quintet multiplicity and CASPT2 and MRCI calculations of the splittings between the singlet-quintet and triplet-quintet multiplicities. These PESs have been tested against cross section and rate coefficient measurements in the thermal**[2]** and subthermal**[3]** ranges, obtaining a good agreement (aprox. 10%). In addition, the role of the PESs for ultracold collisions in a magnetic field has been analyzed**[4]**.

Results mentioned above will be briefly highlighted and the rest of the presentation will focus on discussing the nature of the bonding in the oxygen dimer, trimer and tetramer. For the dimer, we have performed accurate bound states calculations**[5]** and, despite the binding energy is typical of a van der Waals dimer (approx. 100 cm^{-1}), it involves some strength of exchange interactions. For the trimer and specially for the tetramer in its singlet state, multiconfigurational *ab initio* calculations find an incipient chemical bonding at very short cluster sizes that leads to a softening of the repulsive wall**[6]**. We show that these findings are consistent with the structure and other observations of the high pressure (10-90 GPa) diamagnetic ε phase of oxygen.

References:

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