Abstract Submitted
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Resonating Valence Bond wave function with molecular orbitals: first application to dimers[1] SANDRO SORELLA, SISSA and DEMOCRITOS, Via Beirut n.2 34014, Trieste, Italy., SAM AZADI, SISSA, Via Beirut n.2 34014, Trieste, Italy, MARIAPIA MARCHI, SISSA and DEMOCRITOS, Via Beirut n.2 34014, Trieste, Italy, MICHELE CASULA, Centre de Physique Théorique, Ecole Polytechnique, CNRS, 91128 Palaiseau, France — We introduce a method for accurate quantum chemical calculations based on a single determinant wave function, the Antisymmetrized Geminal Power (AGP), and a real space correlation factor (the so called Jastrow factor), that can be efficiently sampled by means of standard quantum Monte Carlo techniques. This allows to obtain a very accurate description of the chemical bond even in extremely difficult cases (such as Be_2, N_2 and C_2) where strong dynamical correlations and/or weak vdW interactions are present. The method is based on a constrained variational optimization, obtained with an appropriate number n of molecular orbitals in the AGP wavefunction. It is shown that the most relevant dynamical correlations are correctly reproduced, once n is univocally determined by the requirement to have size consistent results upon atomization to correlated Hartree-Fock Slater determinants in presence of the Jastrow factor. We apply this method to the Iron dimer molecule and obtain an accurate description of the ground state energy and excitations of this molecule, which is compatible with the experimental findings.

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