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Studying hydrogen bond by Quantum Monte Carlo: binding energy and dispersion curve of the water dimer LEONARDO SPANU, SISSA-ISAS Trieste, Italy; Dept. of Chemistry UC Davis, FABIO STERPONE, LUCA FERRARO, Caspur Roma, Italy, SANDRO SORELLA, SISSA-ISAS Trieste, Italy, LEONARDO GUIDONI, Univ. La Sapienza Roma, Italy — We present a variational MonteCarlo (VMC) and lattice regularized diffusion MonteCarlo (LRDMC) study of the binding energy and dispersion curve of the water dimer. One the aim of the present work is to investigate how the bonding of two water molecules, as a prototype of the hydrogen-bonded complexes, could be described by a JAGP wave function, an implementation of the resonating valence bond idea.Using a pseudopotential for the inert core of the Oxygen, with a full optimization of the variational parameters, we obtain at the VMC level a binding energy of -4.5(0.1) Kcal/mol, while LRDMC gives -4.9(0.1)Kcal/mol (exp. 5 Kcal/Mol). The calculated dispersion curve reproduces both at the VMC and LRDMC level the miminum position and the right curvature.The quality of the WF gives us the possibility to dissect the binding energy in different contributions by appropriately switching off determinantal and Jastrow terms in the JAGP: we estimate the dynamical contribution to the binding energy of the order of 1.4(0.2) Kcal/Mol whereas the covalent one about 1.0(0.2) Kcal/Mol. JAGP reveales thus a promising WF for describing systems where dispersive and covalent forces play an important role

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