Structures and properties of (bio)molecules from Quantum Monte Carlo

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In this contribution I will present an overview of recent applications of Variational Monte Carlo techniques based on the Jastrow Antisymmetrised Geminal Power (JAGP) wave function [1] to molecules in which the electron correlation plays an important role. The compactness of the JAGP ansatz and the possibility to fully optimize all variational parameters (including the exponents of the Gaussian primitives) allow us to obtain with an affordable computational cost an accurate determination of ground state geometries, vibrational properties, transition state structures, electronic densities, diradical and radical states, and polarizabilities [2,3]. Biomolecular applications include the spectral tuning of the Retinal chromophores in Rhodopsin (see picture), the role of the bond length alternation in carotenoids, and the properties of di-nuclear transition metal complexes [4].

