

# Water in Proteins: a Car-Parrinello Investigation

Paolo Carloni

*International School for Advanced Studies, Trieste, Italy*

The properties of water molecules confined in enzyme cavities are poorly understood, yet water plays often a crucial role in molecular recognition, ligand binding and biological function. Here we will present results from Car-Parrinello [1] and Car-Parrinello/molecular mechanics [2] simulations on water present in the active sites of a variety of hydrolytic enzymes [3–5]. We find that water is rather polarized by the environment and that there is a subtle interplay between protein polarization and biological function. We conclude that force-field based methodologies, which are widely used in biomolecular modeling, may encounter difficulties in describing structure and energetics of water in enzymatic systems.

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