The protein is the key: the unique chemistry of biological pigments revealed by a multiscale strategy

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Molecular pigments behave differently when they are embedded in a protein. The electrostatic fields acting in the protein cavity and the (mutual) interactions with the nearby residues can in fact largely affect the nature and the relative energy of pigments' electronic states. Moreover, their conformational space and vibrational motions can be strongly modified. All these effects finally lead to a new chemistry which is at the basis of some of the most important biological functions. The molecular mechanisms determining such a new behavior can only be revealed by computational approaches which are able to couple the structural, electronic and dynamic properties of the pigments and the embedding protein. In this talk, examples of this multiscale modeling will be discussed for biological pigments present in plants and bacteria.