Séminaire :

« Hybrid VB/MM - a Valence Bond ride through classical landscapes »

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The growing demand for realistic methods that would calculate chemical reactions in biological systems resulted with the development of hybrid quantum mechanical (QM) molecular mechanical (MM) schemes. Recent years have proven schemes that are based on concepts from valence bond (VB) methodology, to be beneficial for the description of enzyme catalysis and reactivity. The development of a new hybrid (QM/MM) method where the QM part is treated by ab initio Valence Bond (VB) theory will be presented. This VB/MM method has the advantages of Empirical VB (EVB) methodology but should provide better accuracy and does not rely on empirical parameterization for the quantum part. The validity of the method will be shown to be successful in several examples.