A hierarchy of embedding approaches for the study of molecular properties

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With the rampant development of theoretical chemistry, so have the demands on the field increased. Today, one expects calculations to provide accurate predictions on day-to-day lab experiments. However, even though the numbers may fit, caution should be taken. The simulations are still far from the time and size scales of the chemical mechanisms under study. One ever ongoing task in the field is then to extend the application range of the toolbox of methods. Our take at the problem has been to make use of hybrid QM/QM and QM/MM approaches, which allow one to target specific regions of the system, such as the active site in an enzyme.

In this talk an overview will be given on different strategies for the calculation of extended systems. Applications include the study of enzymatic reaction mechanisms (Mo-enzymes), the calculation of UV-Vis spectra of transient species and the conformational properties of synthetic beta-peptides.