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S E M I N A I R E

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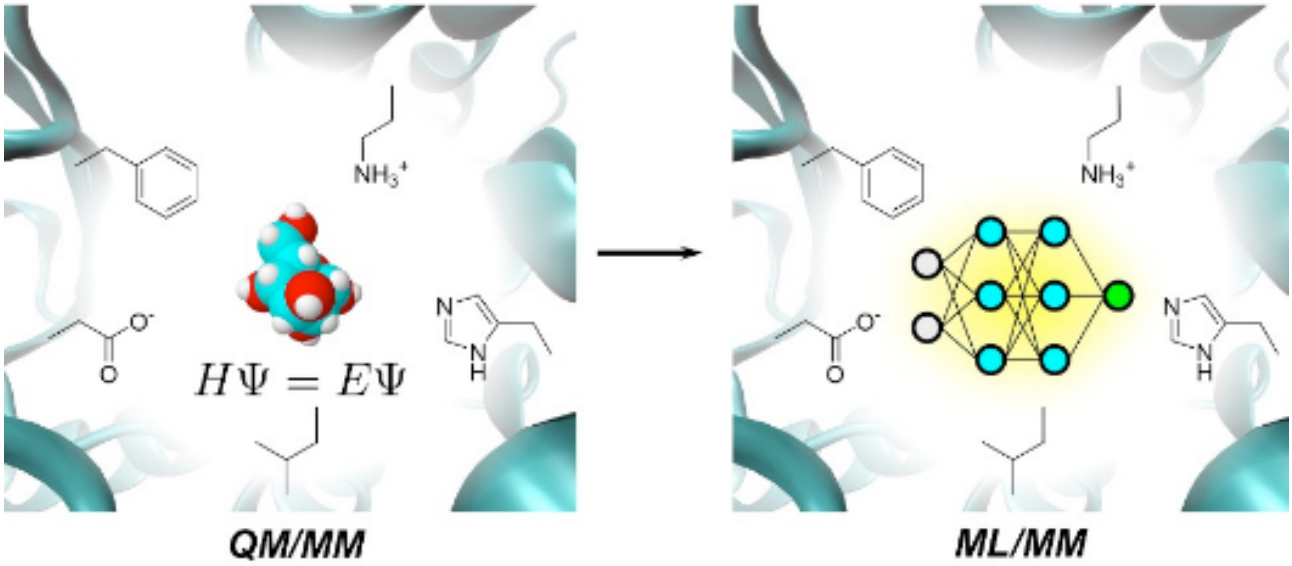
« First steps towards "ML/MM": embedding scheme suitable for machine learning potentials »



Modern computational chemistry relies on precise molecular potentials based on quantum-mechanical (QM) calculations. However, their computational cost is too large even for systemswith only hundreds of atoms. This is an issue for condensed phase systems (biocatalysts,materials etc.) where the number of atoms is often much larger. This problem led to developmentof multiscale models that use a QM potential only for the part of the system where electronicchanges take place, while treating the rest with cheap Molecular Mechanics (MM) forcefields.However, the cost of QM/MM simulations is still dominated by the QM method, making thetimescales needed in some applications beyond reach.An alternative approach, rapidly gaining popularity, is to fit a molecular potential usingMachine Learning (ML) techniques. A trained ML potential provides results much faster than QM,without significant loss in precision. However, ML potentials are still inferior to MM in terms ofcomputational cost. Therefore, a multiscale “ML/MM” scheme, with ML only being employed for thereactive part of the system, would offer huge savings of computer time. Unfortunately, standardapproaches for embedding a QM region into an MM environment are not applicable for ML. I amgoing to present the on-going efforts to develop an embedding scheme that aims to solve thisissue and enable highly accurate hybrid simulations of condensed phase systems at computationalcost comparable to MM

Jeudi 24 mars à 14h30
Salle de conférence