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Multiscale modelling of chemical systems on HPC and quantum computers

Tuesday, 2 December 2025 12:00 (20 minutes)

Multiscale quantum mechanical/molecular mechanical (QM/MM) techniques are a well established approach for simulating chemical reactivity including a realistic description of the surrounding environment. The ChemShell project is a leading software package for performing QM/MM simulations, developed at the UK's Daresbury Laboratory and collaborating research groups around the world. The latest Python-based, open source version of ChemShell maintains a strong emphasis on performance on high performance computers and is widely applicable across a range of research areas from enzyme modelling to materials chemistry. In this talk, recent developments in ChemShell are explored focussing on their computing aspects, including complex workflows targeting exascale calculations through the UK's ExCALIBUR programme, and efforts towards integrating HPC with emerging quantum computing technology in multilayer embedding schemes.

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