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Unbiased QM/MM approach using accurate multipoles from a linear scaling DFT calculation with a systematic basis set STEPHAN MOHR, Barcelona Supercomputing Center, CEA Grenoble, LUIGI GENOVESE, CEA Grenoble, LAURA RATCLIFF, Argonne Leadership Computing Facility, MICHEL MASELLA, CEA Saclay — The quantum mechanics/molecular mechanis (QM/MM) method is a popular approach that allows to perform atomistic simulations using different levels of accuracy. Since only the essential part of the simulation domain is treated using a highly precise (but also expensive) QM method, whereas the remaining parts are handled using a less accurate level of theory, this approach allows to considerably extend the total system size that can be simulated without a notable loss of accuracy. In order to couple the QM and MM regions we use an approximation of the electrostatic potential based on a multipole expansion. The multipoles of the QM region are determined based on the results of a linear scaling Density Functional Theory (DFT) calculation using a set of adaptive, localized basis functions, as implemented within the BigDFT software package. As this determination comes at virtually no extra cost compared to the QM calculation, the coupling between QM and MM region can be done very efficiently. In this presentation I will demonstrate the accuracy of both the linear scaling DFT approach itself as well as of the approximation of the electrostatic potential based on the multipole expansion, and show some first QM/MM applications using the aforementioned approach.

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