Advanced Sampling and Quantum Effects with CP2K and i-PI

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CP2K provides state-of-the-art electronic structure calculation techniques, that are both efficiently implemented and scalably parallelized. I will discuss how it can be used in synergy with the i-PI universal force engine to achieve efficient sampling of different ensembles, including also simulations that treat rigorously the quantum mechanical nature of the nuclei. An uncompromising description of atomistic systems, treating both electron and nuclei quantum mechanical, can now be obtained with minimal computational overhead and no implementation burden.