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Quantum-Classical Adaptive Coupling in Grand-Canonical like Adaptive Resolution Simulations[1] ANIMESH AGARWAL, LUIGI DELLE SITE, Institute for Mathematics, Arnimallee 6, D-14195, Freie Universitat, Berlin, Germany — We have extended the recently developed Grand Canonical AdResS (GC-AdResS) [1,2] to quantum-classical adaptive coupling where the quantum delocalisation of an atom is described by the path integral formalism. Compared to standard adaptive coupling approaches [3], the advantage of GC-AdResS is that there is no need to obtain a coarse-grained model that correctly reproduces the structural and thermodynamic properties of a full PI (path integral) system, thereby eliminating the need to run a full PI simulation before starting the adaptive simulation. In this context, we have shown that spherical molecules described by a simple generic WCA potential in the coase-grained region, act as a particle reservoir for the PI region. The resulting Grand Canonical set up is such that the structural and dynamical properties of quantum flexible water models in the PI subregion in AdResS are consistent with the properties obtained in the same subregion in full PI simulations.

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[2] A. Agarwal, H. Wang, C. Schütte and L. Delle Site, J.Chem.Phys. **141**, 034102 (2014)
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