

Proton transfer in bulk water using the full adaptive QM/MM method: Integration of solute- and solvent- adaptive approaches

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Supporting Information

Figure S1. Potential of mean force in aqueous phase of proton transfer obtained with SCMP simulation with the EPI parameter $c = 0.2$. Here, the horizontal axis represents distance between the oxygen atom O* nearest to the QM center and the second nearest oxygen O'. The vertical axis represents the transferred hydrogen displacement $\delta = R_{O'H} - R_{O^*H}$.

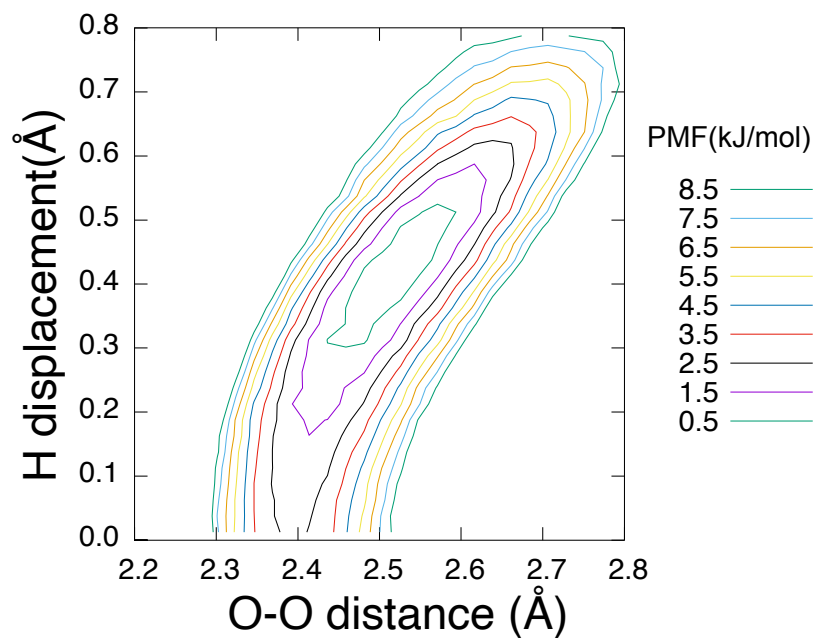


Figure S2. Mean square displacement (MSD) of the EPI. The black lines represent the result with $c = 0.0$ which were averaged over 15 independent 100ps-MD simulations. The red lines represent the fitting line with $y = ax + b$.

