Supporting information for:

Accurate Quantum Mechanics/Molecular Mechanics Simulation of Aqueous Solutions with Tailored Molecular Mechanics Models

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1 Methanol in water

The PM6-DH+ / PM6-DH+-EFF simulations of MeOH in water result in the C-O radial distribution in S1. The first solvation peak is in perfect agreement with the peak location observed in two different ab initio simulations.[S1,S2] We do observe a discrepancy in the second solvation peak (5.5 Å), which is found at a smaller distance than in the HF simulations (6.5 Å).[S1] The DFT results[S2] do not contain the second peak within the limited simulation cell.
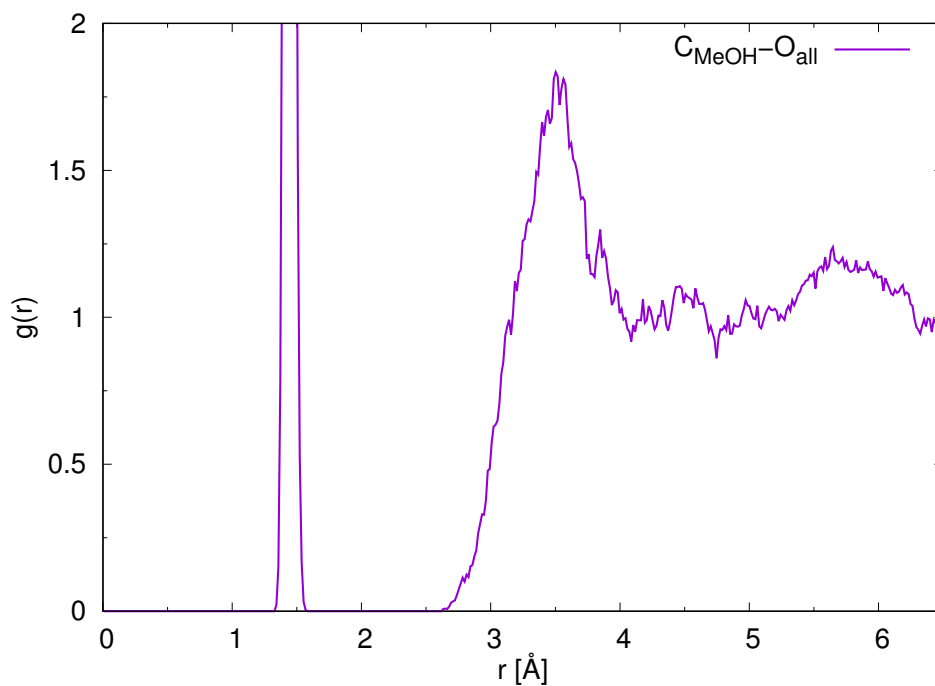
Figure S1: Radial distribution of all oxygen atoms (O_{all}) around carbon atom in the methanol (C_{MeOH}) from the Abrupt adaptive QM/MM simulation.

References

(S1) Moin, S. T.; Hofer, T. S.; Randolf, B. R.; Rode, B. M. *Journal of Computational Chemistry* **2010**, *32*, 886–892.

(S2) van Erp, T. S.; Jan, M. E. *Chemical Physics Letters* **2001**, *333*, 290–296.