

Electronic Supplementary Information

Elucidating the Role of Solvents in Acid Catalyzed Dehydration of Biorenewable Hydroxy-Lactones

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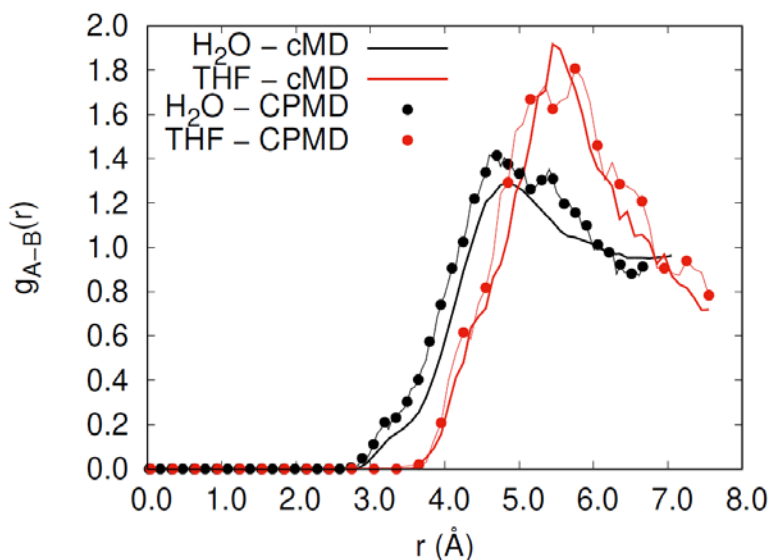


Figure S1: Comparison of radial distribution function (RDF) obtained from classical molecular dynamics (cMD) and Car-Parrinello molecular dynamics (CPMD) for HML-H⁺ complex in bulk water and THF. The RDF is calculated using center of mass of HML-H⁺ complex, oxygen atom of water molecules, and center of mass of THF molecules.