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# Ab initio QM/MM dynamics of anion–water hydrogen bonds in aqueous solution

Anan Tongraar [a,*], Bernd Michael Rode [b]

[a] *School of Chemistry, Institute of Science, Suranaree University of Technology, 111 University Avenue, Muang Dist., Nakhon-Ratchasima 30000, Thailand*
[b] *Department of Theoretical Chemistry, Institute of General, Inorganic and Theoretical Chemistry, University of Innsbruck, Innrain 52a, A-6020 Innsbruck, Austria*

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**Abstract**

Dynamical properties of $F^-$–water and $Cl^-$–water hydrogen bonds in aqueous solution have been studied by ab initio QM/MM molecular dynamics simulations, in which the whole first hydration sphere of the anion was treated at Hartree–Fock level using D95V+, 6-31+G and D95V++ basis sets for $F^-$, $Cl^-$ and water, respectively. According to a detailed analysis of the bond distortions and shifts in the corresponding bending and stretching frequencies as well as the mean residence times of water molecules surrounding the ions, $F^-$ clearly acts as a 'structure-maker', while $Cl^-$ solvation leads to a more flexible structure with frequent re-arrangements of the hydrogen bonds.