Unraveling the Hydration Properties of the Ba^{2+} Aqua Ion: the Interplay of Quantum Mechanics, Molecular Dynamics and EXAFS spectroscopy

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Supporting online information

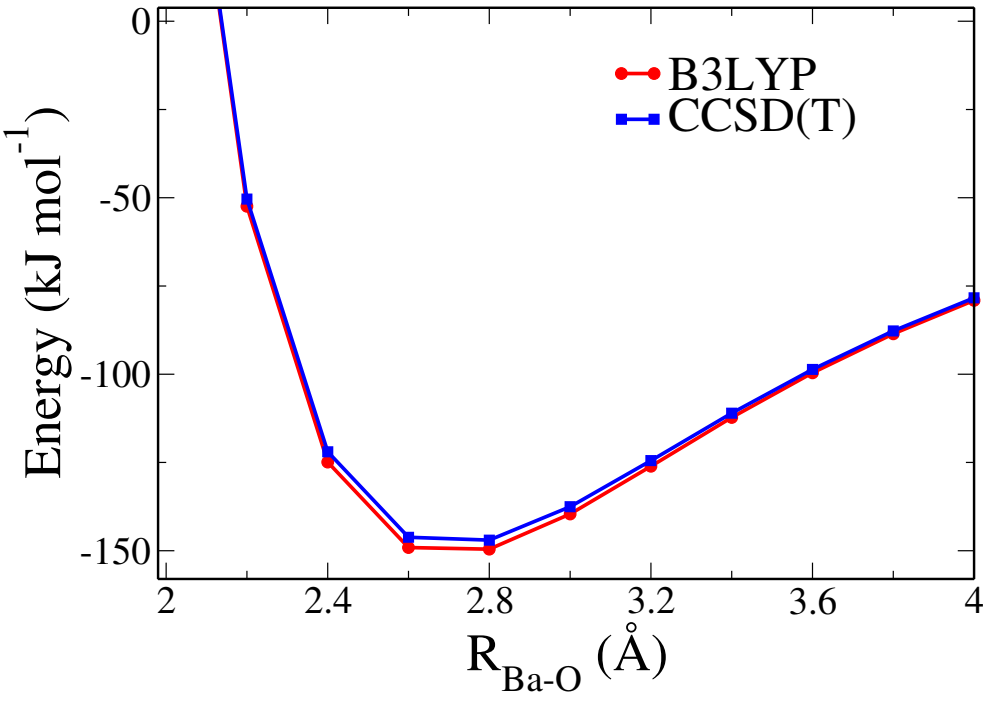

Figure 1S. Ba^{2+}-water interaction energies calculated in vacuum by using DFT with the B3LYP hybrid functional (red circles) and by means of the CCSD(T) method (blue squares). The curves are shown as a function of the Ba-O distances and refer to an anti-dipole orientation of the water molecule with respect to the ion (Ba-O-H angle of 127.7° and all coplanar atoms).

	Parameters	Std. Dev.
A_o (kJ mol^{-1} nm^4)	$3.786{\cdot}10^{-1}$	$1.32\ {\cdot}10^{-2}$
B_o (kJ mol^{-1} nm^6)	$-1.906{\cdot}10^{-2}$	$6.43\ {\cdot}10^{-3}$
C_o (kJ mol^{-1} nm^8)	$-1.445{\cdot}10^{-3}$	$2.55\ {\cdot}10^{-4}$
D_o (kJ mol^{-1} nm^{12})	$3.510{\cdot}10^{-7}$	$1.67\ {\cdot}10^{-8}$
E_o (kJ mol^{-1})	$1.432{\cdot}10^{+6}$	$1.28\ {\cdot}10^{+5}$
F_o (nm^{-1})	$3.645{\cdot}10^{+1}$	1.45
A_h (kJ mol^{-1} nm^4)	$-8.701{\cdot}10^{-2}$	$1.78\ {\cdot}10^{-3}$
B_h (kJ mol^{-1} nm^6)	$5.210{\cdot}10^{-3}$	$1.09\ {\cdot}10^{-4}$
C_h (kJ mol^{-1} nm^8)	$-4.192{\cdot}10^{-5}$	$3.80\ {\cdot}10^{-6}$
D_h (kJ mol^{-1} nm^{12})	$8.124{\cdot}10^{-10}$	$4.22\ {\cdot}10^{-11}$

Table 1S. Ba^{2+}-water interaction parameters and relative standard deviations obtained by the fitting procedure carried out using a charge of 2.0 a.u. on the cation.

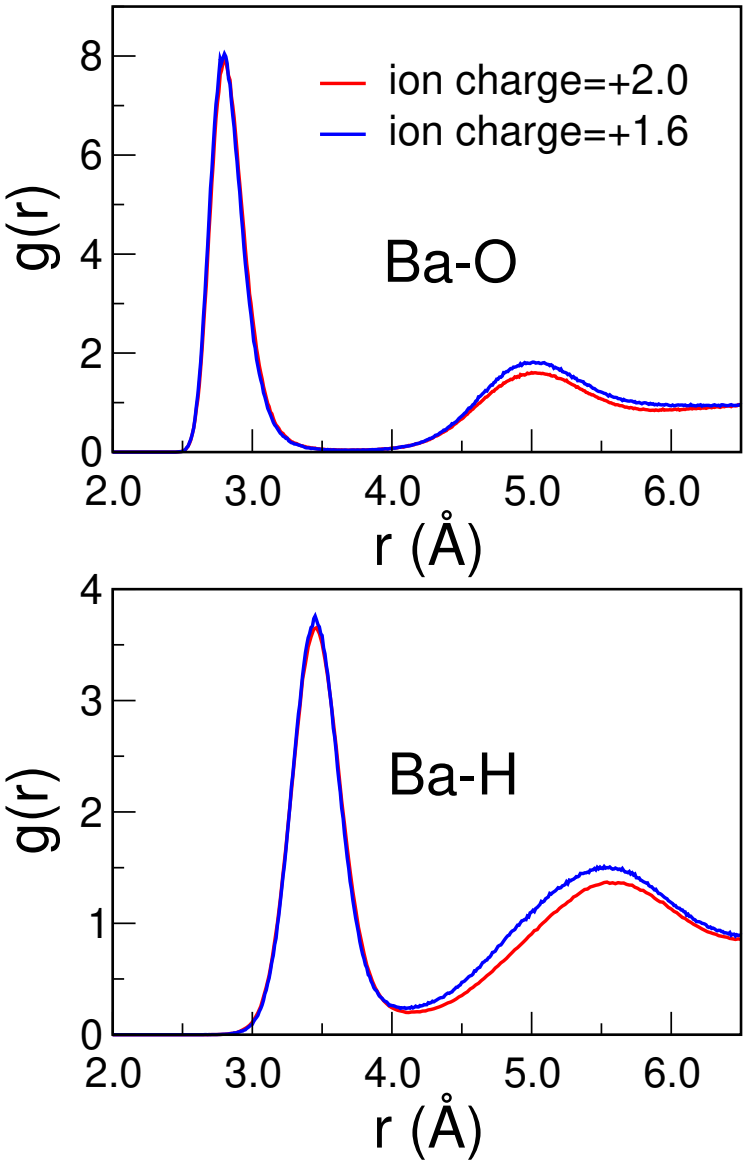

Figure 2S. Comparison of the Ba-O (upper panel) and Ba-H (lower panel) radial distribution functions $g(r)$'s calculated from the MD simulations carried out by using a charge of either 2.0 a.u. (red lines) or 1.6 a.u. (blue lines) on the cation.