Effect of the Zn^{2+} and Hg^{2+} ions on the structure of liquid water

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Supporting Information

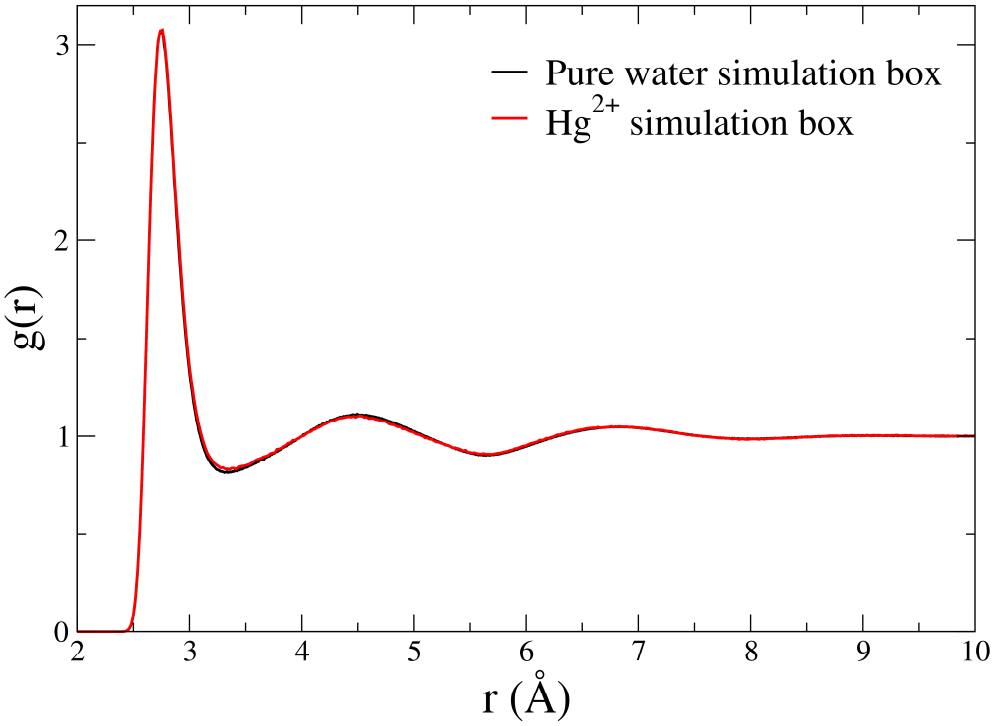

Figure 1S. Comparison of the oxygen-oxygen g(r)'s obtained for pure water (black line) and for the bulk water molecules of MD simulation of Hg^{2+} in water (red line).

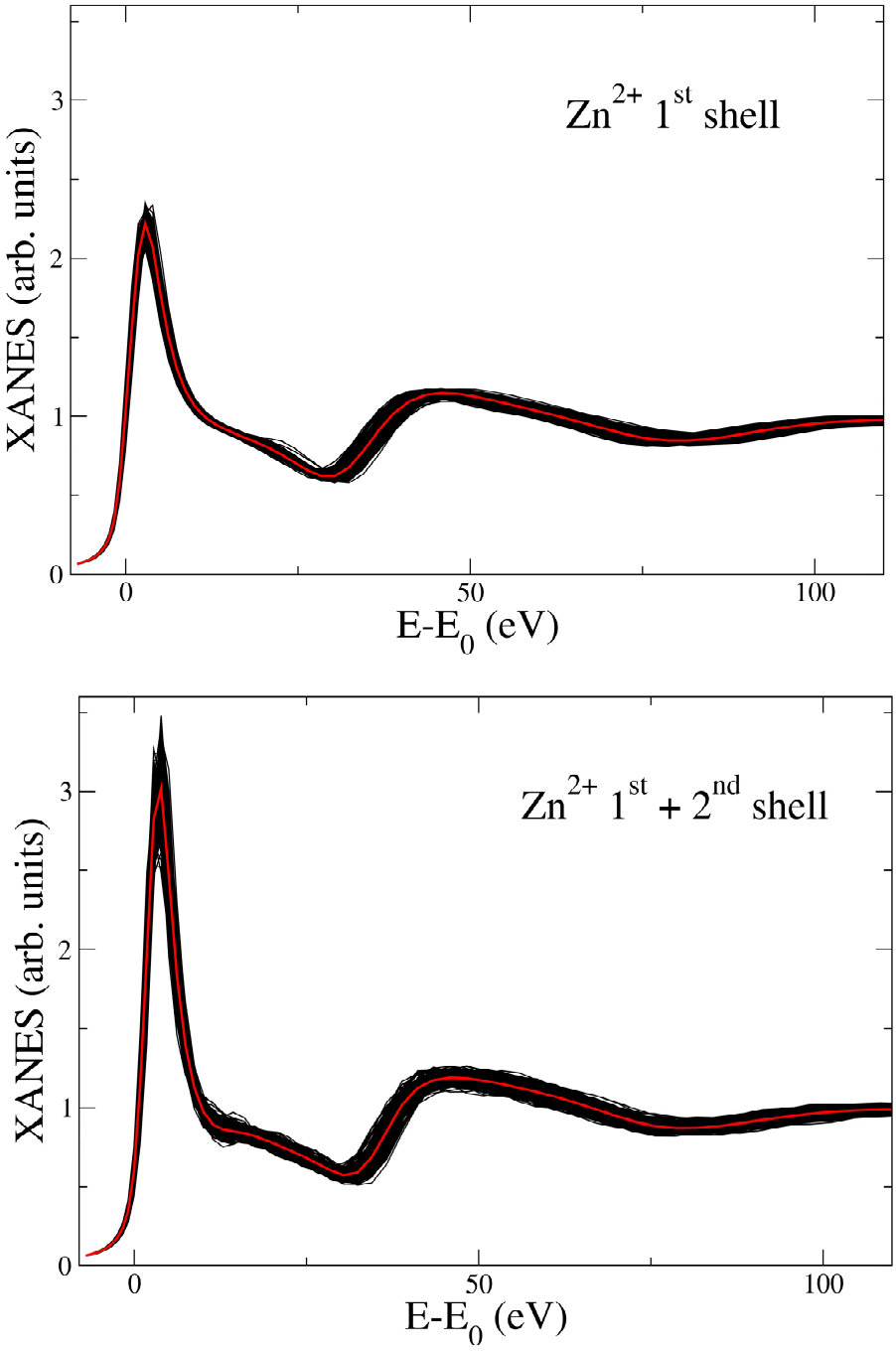

Figure 2S. **(**Upper panel) Comparison of the theoretical XANES spectrum of Zn^{2+} obtained from the MD average including the first hydration shell only (red line) and 200 spectra associated with individual MD configurations (black lines). **(**Lower panel) Comparison of the theoretical XANES spectrum of Zn^{2+} obtained from the MD average including the first plus second hydration shells (red line) and 200 spectra associated with individual MD configurations (black lines).

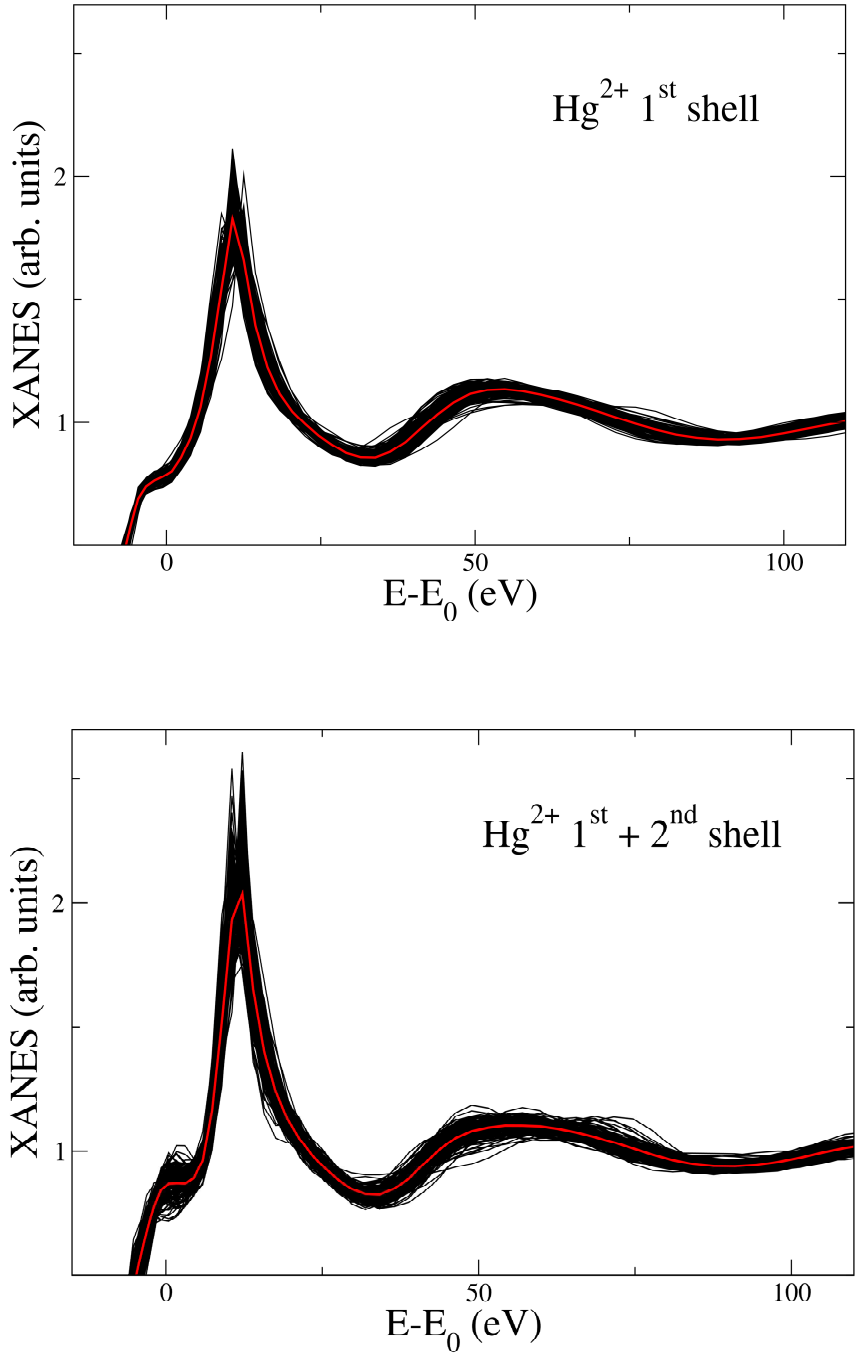

Figure 3S. **(**Upper panel) Comparison of the theoretical XANES spectrum of Hg^{2+} obtained from the MD average including the first hydration shell only (red line) and 200 spectra associated with individual MD configurations (black lines). **(**Lower panel) Comparison of the theoretical XANES spectrum of Zn^{2+} obtained from the MD average including the first plus second hydration shells (red line) and 200 spectra associated with individual MD configurations (black lines).

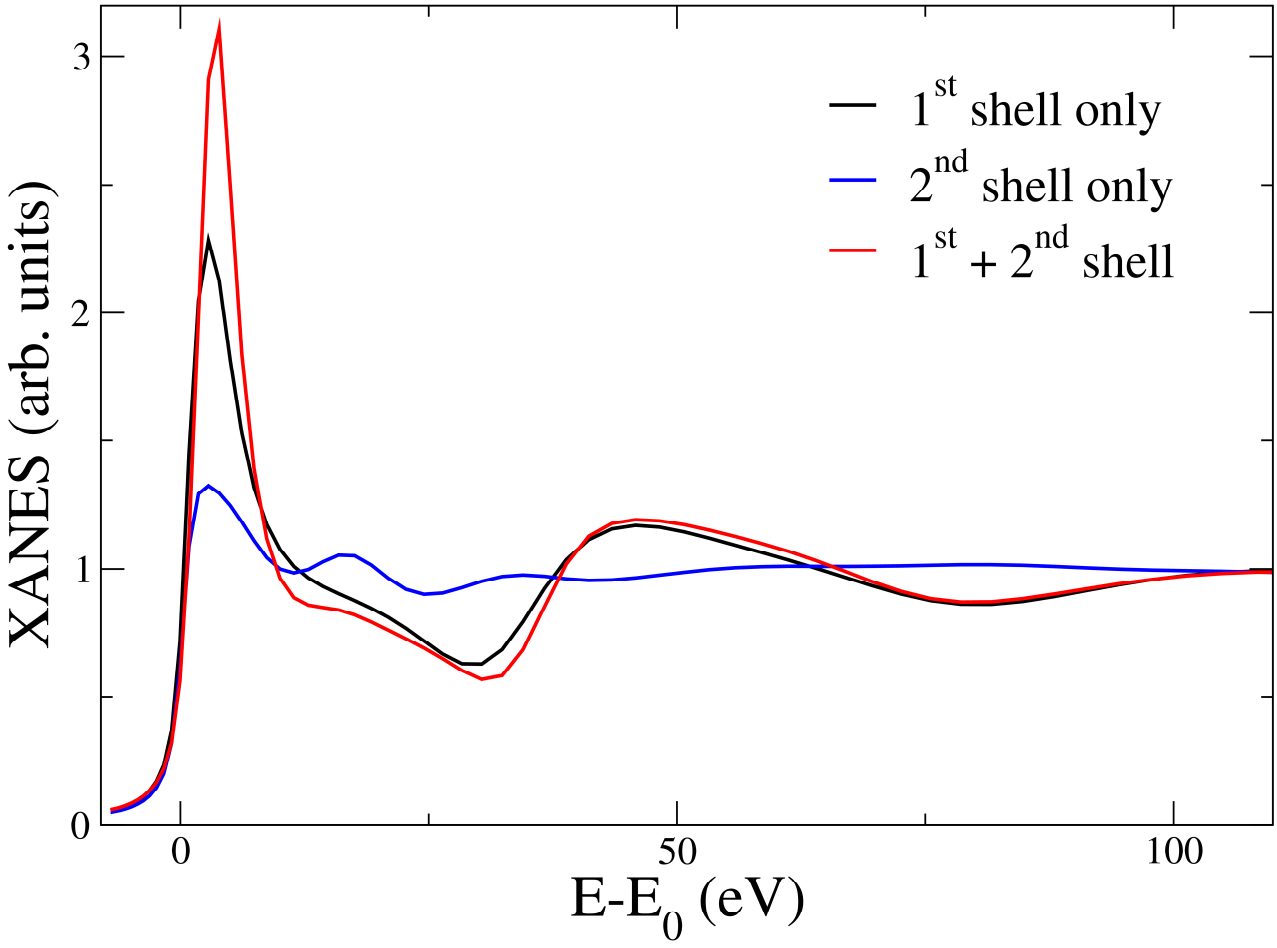

Figure 4S. Comparison of the theoretical XANES spectrum of Zn^{2+} obtained from the MD average including the first hydration shell only (black line), the second hydration shell only (blue line), and the first plus second hydration shells (red line).

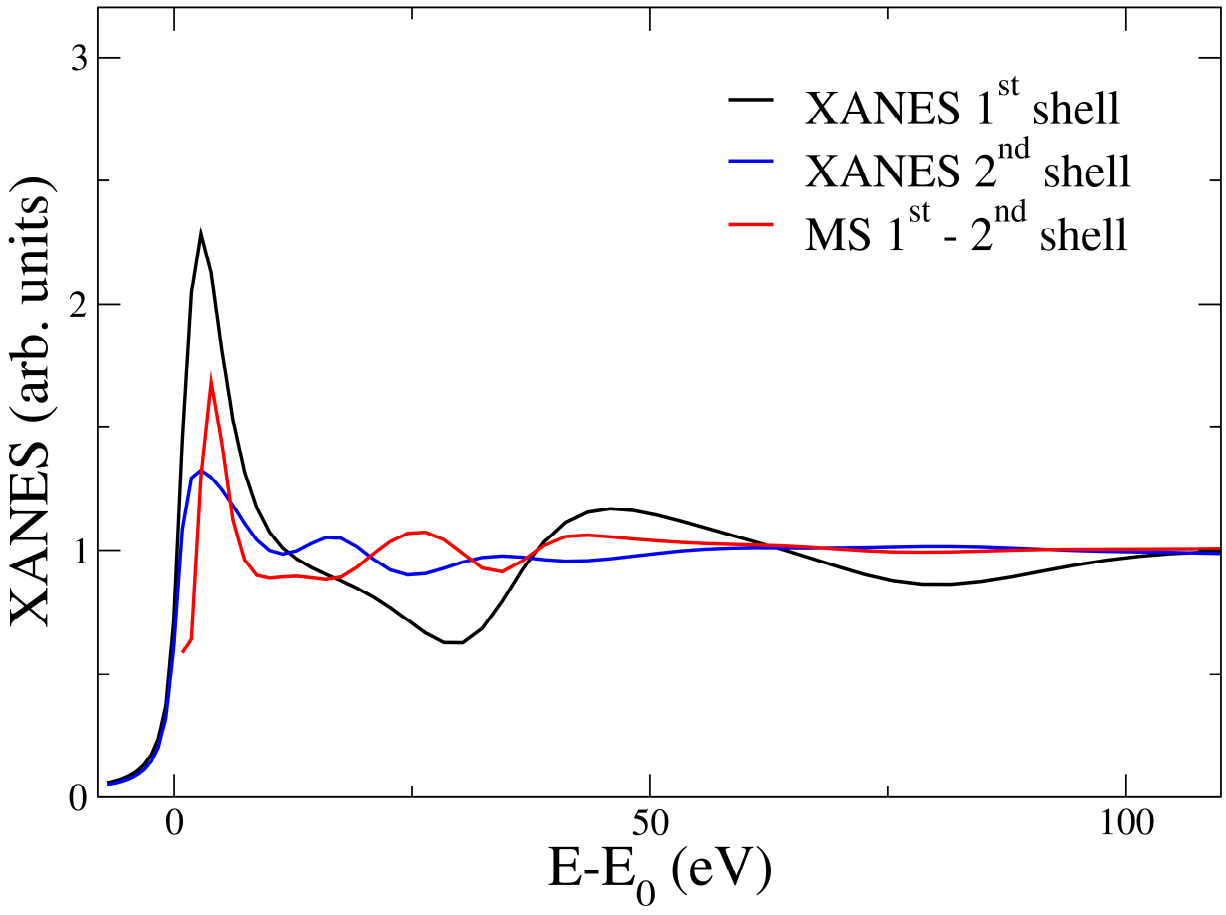

Figure 5S. Comparison of the theoretical XANES spectrum of Zn^{2+} obtained from the MD average including the first hydration shell only (black line), the second hydration shell only (blue line), and the spectrum obtained as the difference between the first plus second hydration shell XANES and the sum of the first hydration shell only and the second hydration shell only spectra (red line). This last spectrum represents the MS contribution associated with Zn-O_1-O_2 paths where O_1 is an oxygen atom of the first hydration shell and O_2 is an oxygen atom of the second hydration shell.