Erratum: Local correlated motions in aqueous solution of sodium chloride [Phys. Rev. Materials 3, 065604 (2019)]

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In the original paper, we inadvertently used an incorrect time axis for the figures and fitting procedures. It was too large by a factor of 2. All the values of time need to be the half of those in the original paper. This influences the timescales in Figs. 2, 4, 6, and 7 and the fitted parameter of τ_1 and τ_2 in Figs. 5 and 6; all the time axes are reduced by a half. The necessary corrections are as follows:

(1) The text on p. 4, left column, last paragraph should be changed to: “At a longer timescale [$t > 0.25$ (rather than 0.5 in the original paper) ps], the addition of salt induces a qualitative change at the first- and the second-neighbor peaks.” and “Therefore, the first-neighbor correlation is dominant in the NaCl aqueous solution at $t > 0.5$ ps.” In addition to the changes in the timescale, we reexamined the energy resolution function. The correct values for τ_G is 0.1 ps and for τ_E is 1 ps on p. 2.

(2) The text on p. 6, left column, last paragraph of Sec. III B. should be changed to: “The fact that all the decay curves intersect at $t = 0.14$ ps supports that the spectra are decomposed into the linear combination.” The text on p. 6, left column, the paragraph next to Eq. (10) should be changed to “At a short time ($t < 0.3$ ps), positive correlation peaks are observed” The text on p. 6, right column, last paragraph should be changed to: “due to a contamination of termination errors in the Van Hove functions at a short time, particularly at $t < 0.1$ ps, [$\cdots$] approximated by a two-step relaxation, $I(t) = 1.5 \exp[-(\frac{t}{0.16 \text{ ps}})^{1.7}] = 0.6 \exp(-t/1.0 \text{ ps})$ as shown by the solid line in Fig. 7 (bottom). The first term is almost identical to that of pure water ($\tau_1 = 0.16$ ps), except for its amplitude, indicating that the decaying at a short timescale ($t < 0.15$ ps) corresponds to a ballistic, [$\cdots$].”

(3) The text on p. 7, left column, first paragraph should be changed to “that of water-water correlations with a decaying time ~ 1 ps,” The text on p. 7, left column, last paragraph should be changed to “The values of the normalized amplitude remain almost constant for $t < 0.15$ ps.

(4) Timescales of Figs. 2, 4, 6, and 7 should be changed, and the fitting result in Fig. 5 was updated. The complete Figs. 2, 4, 5, 6, and 7 are reprinted here.

The discussion and the conclusions presented in our original paper remain unaffected.

FIG. 2. The Van Hove function of a NaCl aqueous solution. (Top) One-dimensional slice of the Van Hove functions $G(R, t)$ at $0 < t < 1$ ps. (Middle) Intensity map of $G(R, t) - 1$, the color scale of which is shown on the bottom. Left to right: $m = 0$ (pure water), 0.75, 1.5, 2.26, and 3.0 mol/kg.

FIG. 4. Temporal changes in the area of the first-neighbor peak, $A_1(t)$, and the enlarged view (inset): (open circles) pure water, (triangles) $m = 0.75$ mol/kg, (squares) 1.5 mol/kg, (closed circles) 2.26 mol/kg, and (diamonds) 3.0 mol/kg. The shaded areas represent uncertainties of each dataset. The solid and dashed lines represent the linear combination of time evolution for $m = 0$ and 2.26 mol/kg (see the main text).

FIG. 5. Fitting results of the first-neighbor decay. (Triangles) a_1 , τ_1 , p_1 , (diamonds) a_2 , τ_2 , p_2 , and (circles) $A_1(0)$. The error bar is estimated by the standard deviation of the fitting.

FIG. 6. (Top) One-dimensional profiles of $G'(R, t)$ at $0 < t < 1$ ps and (middle) their intensity maps. Their color scale is shown on the right. The molality of the sample is 0.75, 1.5, 2.26, and 3.0 mol/kg from the left to the right. The solid lines, dashed lines, and the dashed-dotted lines in the top figures represent $R = 3.21$ Å ($R_{O_2^-} + R_{Cl^-}$), $R = 2.42$ Å ($R_{O_2^-} + R_{Na^+}$), and $R = 2.8$ Å ($R_{O_2^-} + R_{O_2^-}$), respectively. (Bottom) Time evolution of the peak height at around $R = 3.21$ Å. The solid line shows the result of fitting using two (compressed) exponential functions (see the main text).

FIG. 7. Normalized temporal changes in the area of the third peak, $A_3(t)/A_3(0)$, around $R = 6.8$ Å; (open circles) pure water, (triangles) $m = 0.75$ mol/kg, (squares) 1.5 mol/kg, (closed circles) 2.26 mol/kg, and (diamonds) 3.0 mol/kg. Inset: Dependence of $A_3(0)$ on the molality.