Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Diffusion of molecules in the bulk of a low density amorphous ice from molecular dynamics simulations

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Supplementary Information

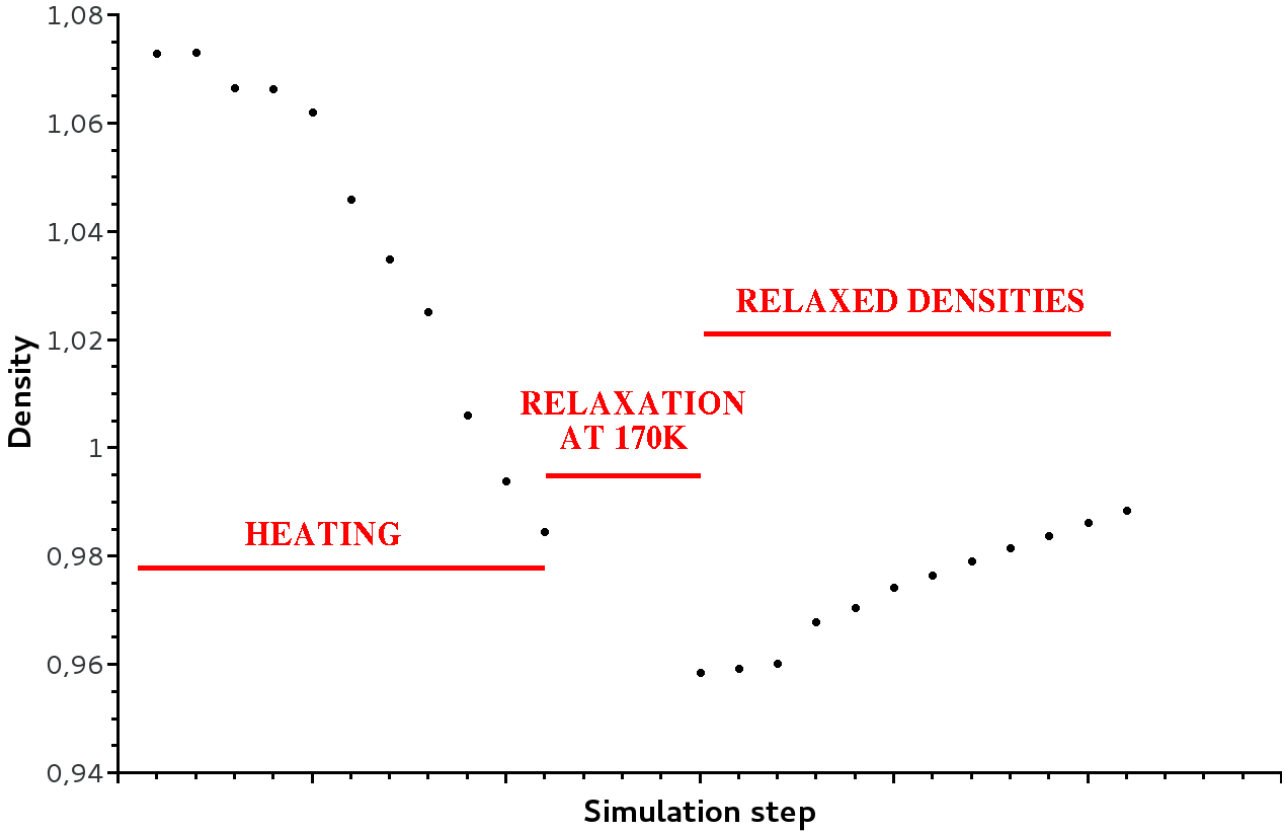

Figure S1: *Calculated densities of the ice during the simulated annealing procedure. Abscise is arbitrary and represents the path along the procedure.*

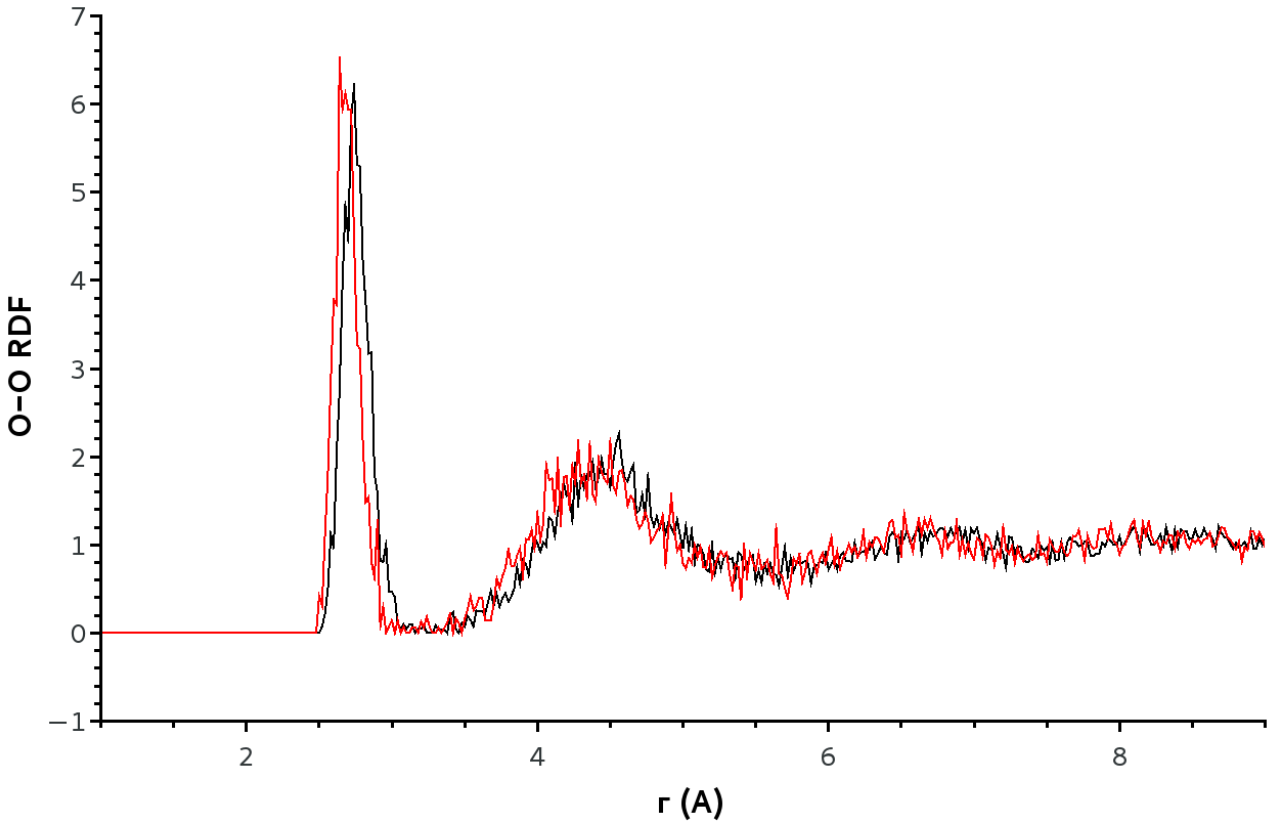

***Figure S2**: Calculated O-O RDF : $g_{OO}(r)$, for the "reference system" (in black) and for the TIP4PQ/2005 ice (in red) at 170K.*

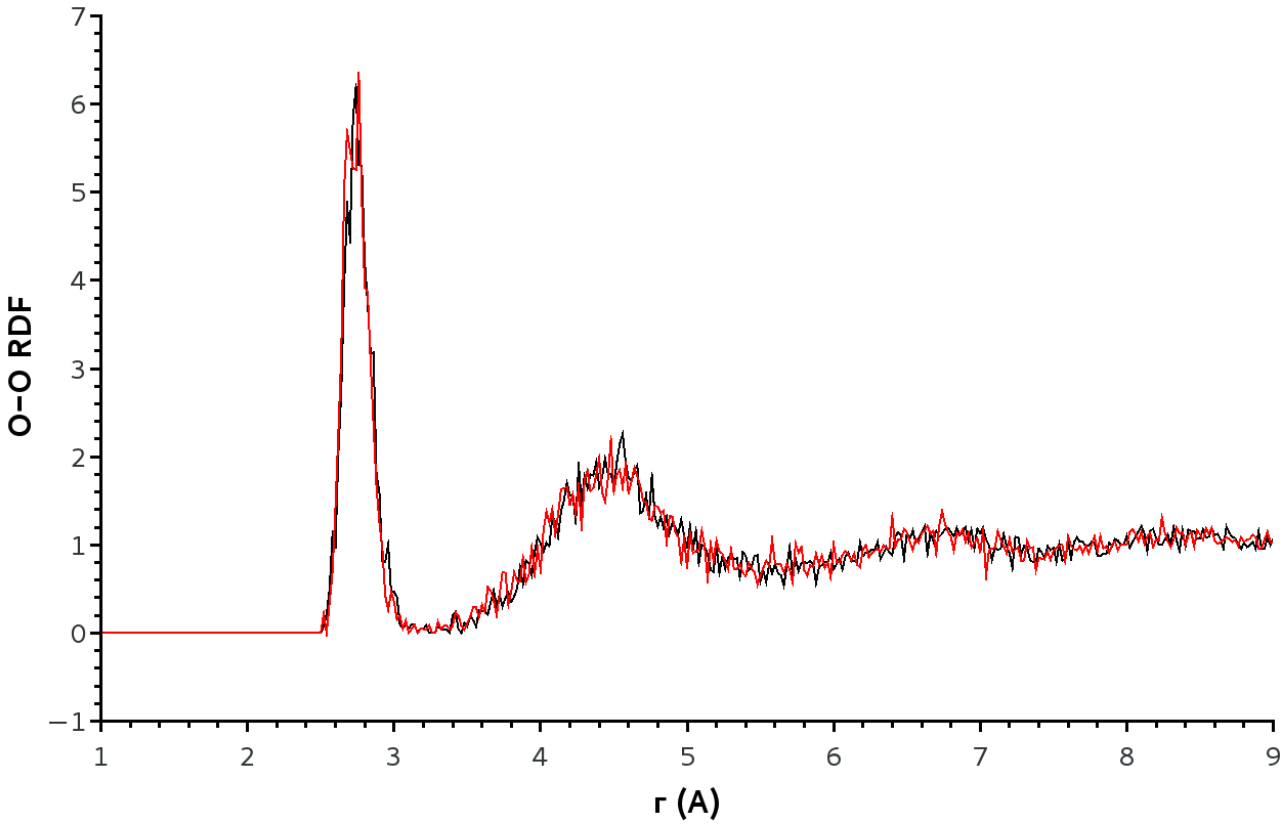

***Figure S3**: Calculated O-O RDF : $g_{OO}(r)$, for the "reference system" for the 360 water molecules box (in black) and for the 540 water molecules box (in red).*

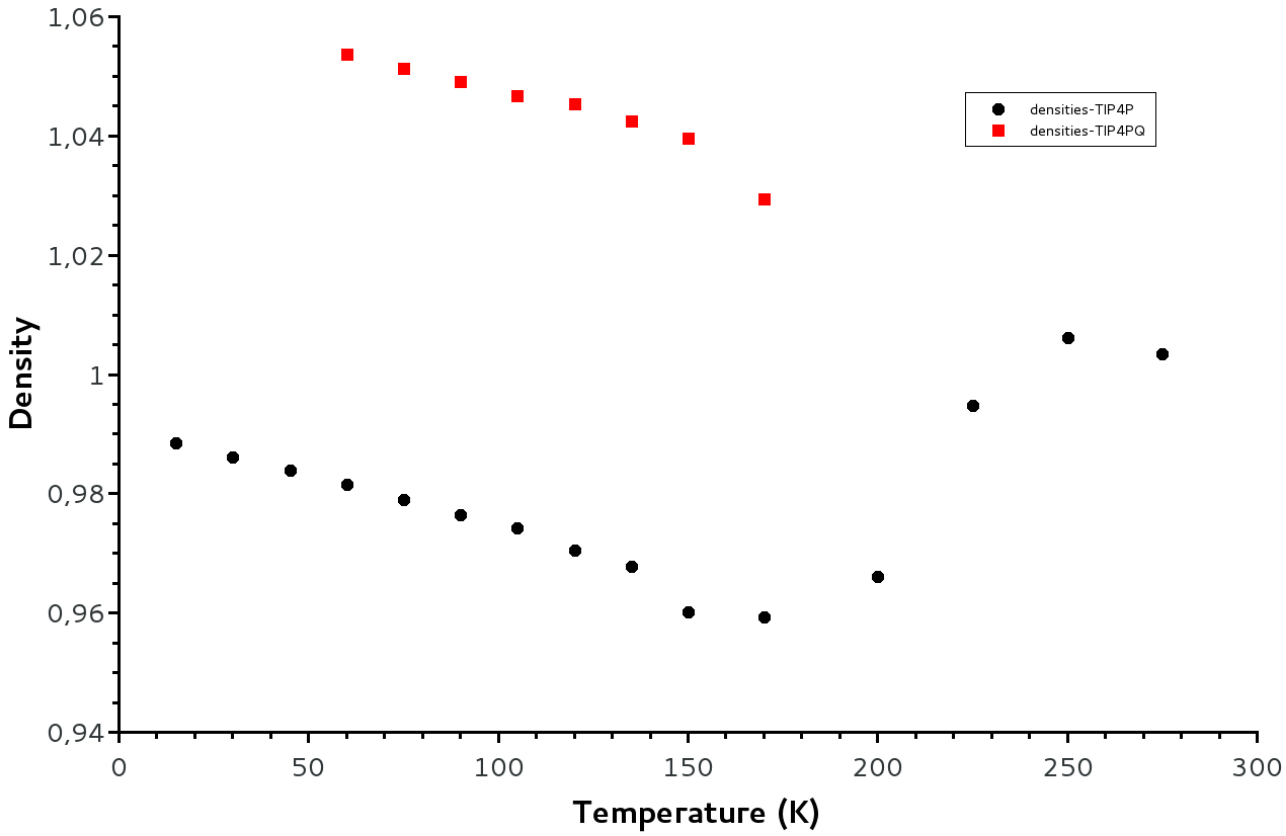

Figure S4: *Density profiles calculated for the equilibrated structures of the "reference system" with the TIP4P model (in black) and with TIP4PQ/2005 model (in red) for temperatures ranging from 90K to 170K.*

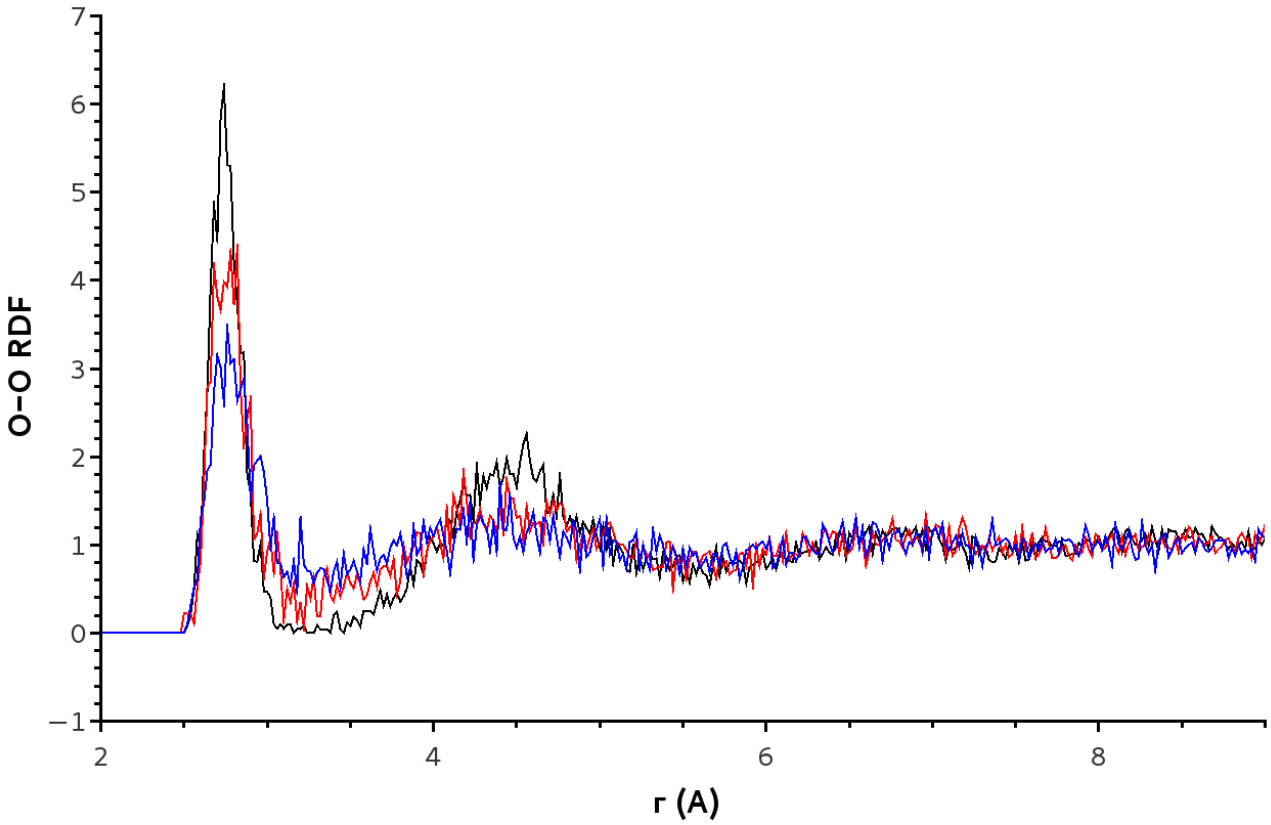

***Figure S5**: Calculated O-O RDF : $g_{OO}(r)$, for the "reference system" for three different temperatures: 170 K in black, 225 K in red, and 275 K in blue.*

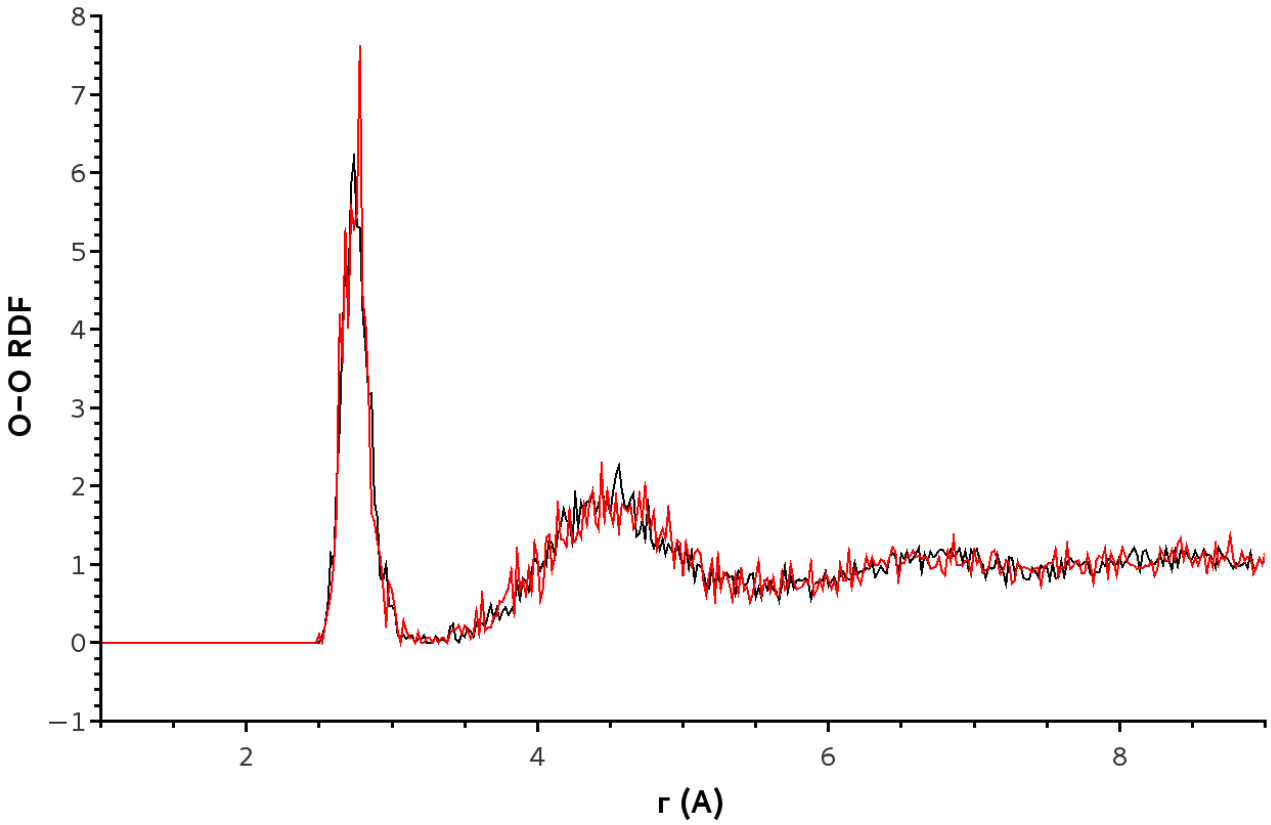

Figure S6: *Calculated O-O RDF : $g_{OO}(r)$, for the "reference system" (in black), and for the system with one solute TIP3P molecule in the TIP4P LDA ice (in red), at 170K.*

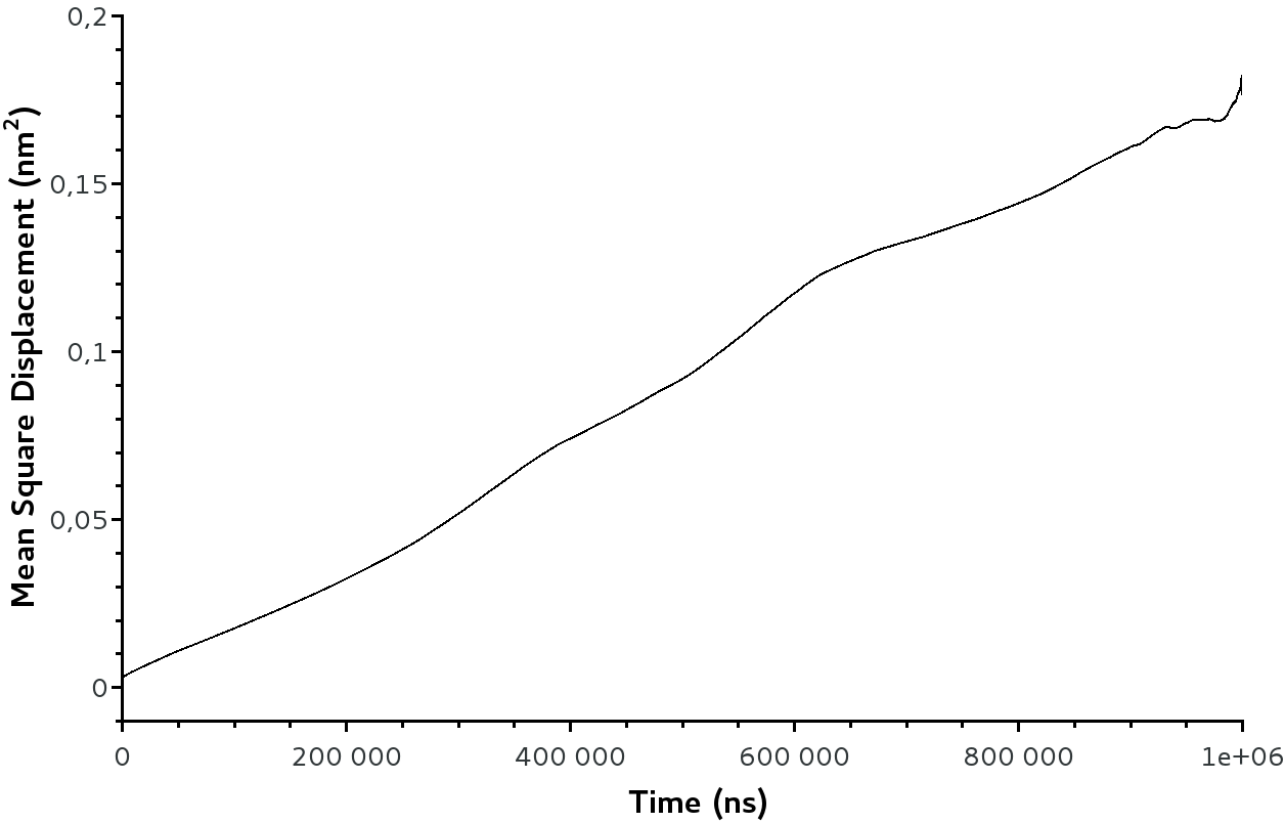

Figure S7: *Water Mean Square Displacements (MSD) for the "reference system" calculated at 170K from a 1 microsecond trajectory*

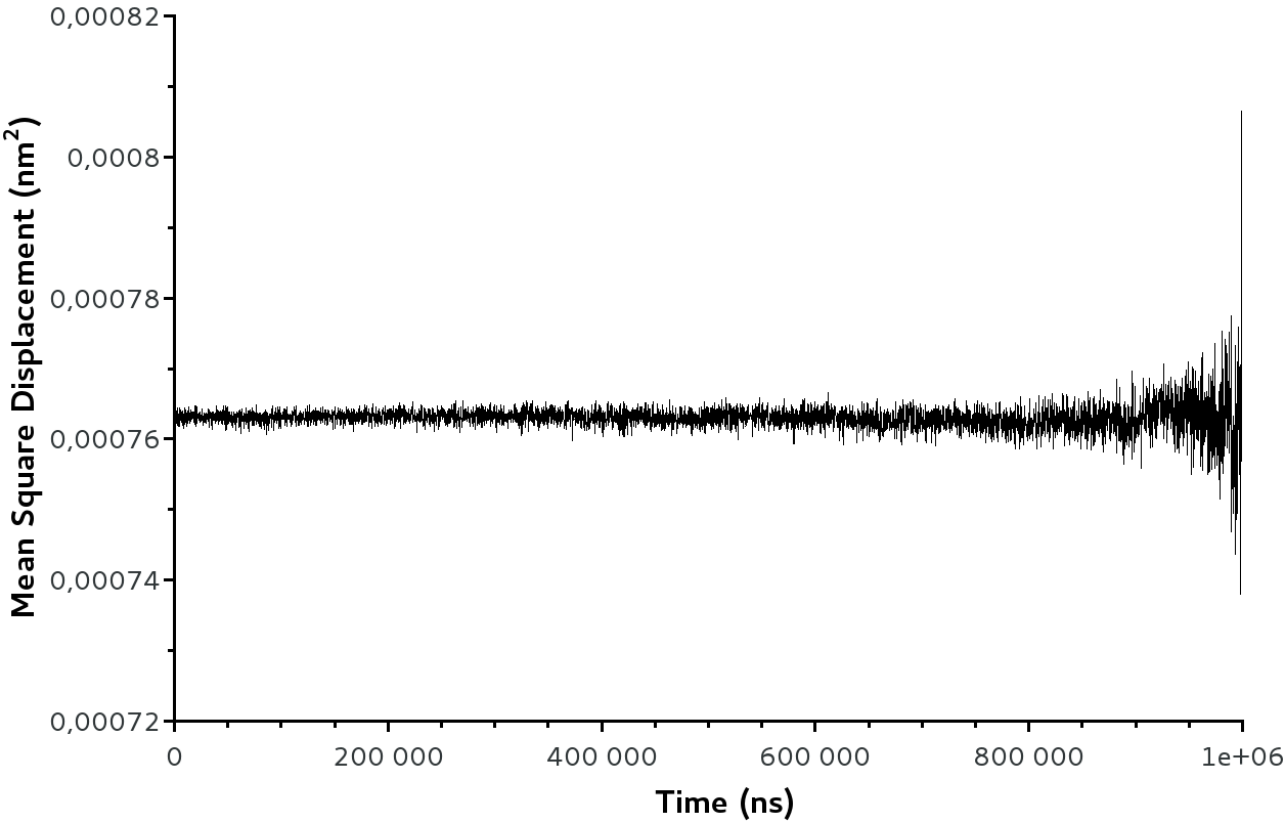

Figure S8: *Water Mean Square Displacements (MSD) calculated at 60K for the "reference system" from a 1 microsecond trajectory*

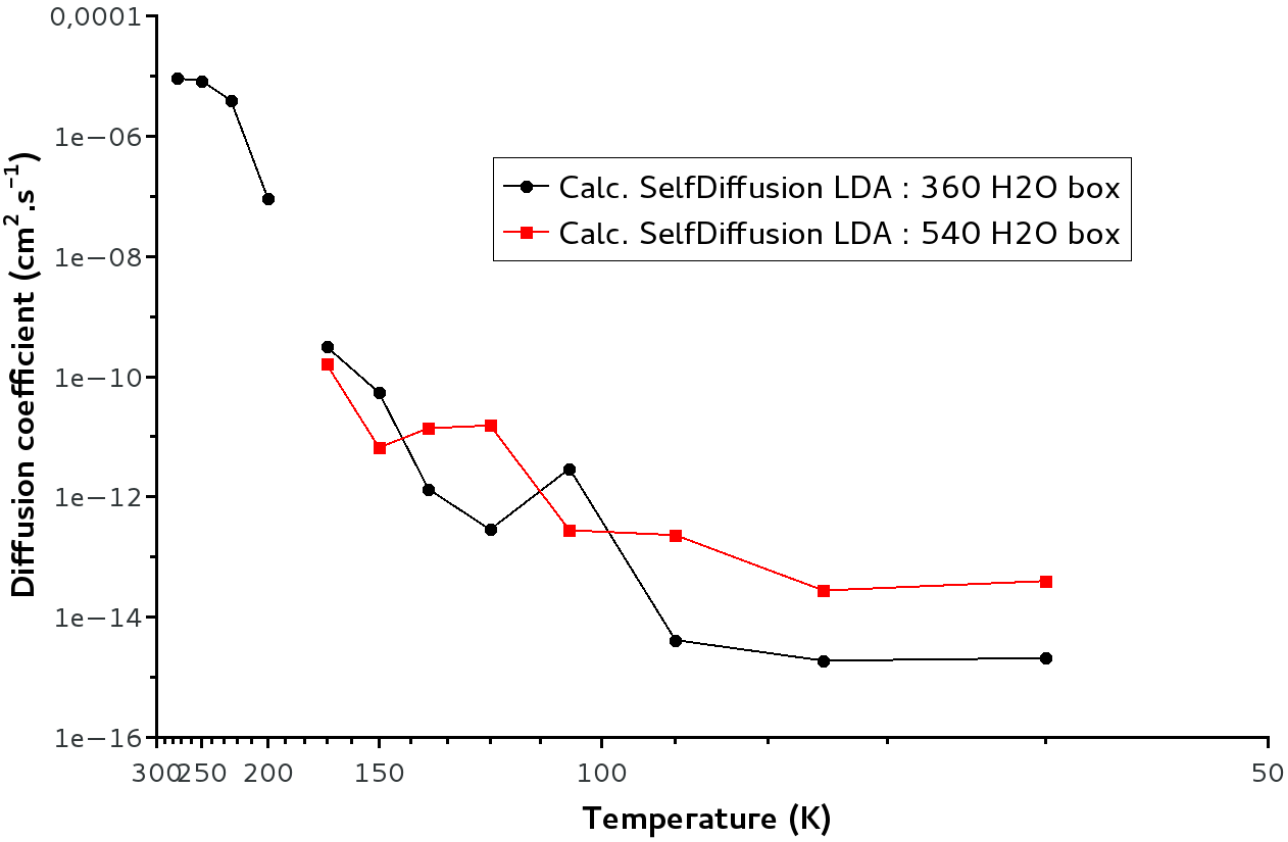

Figure S9: *Water Self-Diffusion coefficients calculated for a LDA ice of 360 water molecules (in black) and 540 water molecules (in red)*