

Supplementary information

Details of the molecular dynamics

Xenon atoms interact via Lennard-Jones potential.

$$U(r) = 4\varepsilon[(\sigma/r)^{12} - (\sigma/r)^6] \quad (1)$$

Potential parameters [1] are $\sigma = 3.94 \text{ \AA}$, $\varepsilon = 0.02 \text{ eV}$. Ion-neutral interaction potential has a form [2]

$$U(r) = (E_0/3)[(R_i/r)^{12} - (R_i/r)^4] = \beta/r^{12} - \alpha/r^4, \quad (2)$$

where $-\alpha/r^4$ represents polarization interaction between the ion and induced dipole. Ion size variation is performed at fixed value of long range attraction parameter α . $\alpha = \alpha_p e^2/2 = 28.8 \text{ eV \AA}^4$. α_p is xenon polarizability, e is the ion charge. Xenon modeling is performed at $T=163 \text{ K}$ and $\rho = 3 \text{ g/cm}^3$.

One ion is added to 5324 xenon atoms. Numerical integration is carried out via Verlet integration scheme. A time step is 3 fs. System is brought to the chosen temperature using Langevin thermostat with dumping constant of 1 ps. The calculation of the diffusion coefficient is carried out in NVE ensemble. Total time of the simulation in NVE ensemble is 8.4 ns.

A polar liquid of choice is water. Water simulation is performed with two different potential models. First model is SPC/E [3]. The ion potential [4,5] is taken in the form of the Buckingham potential superimposed to the Coulomb potential

$$U(r) = A \exp(-r/r_0) - C/r^6 + kq_1q_2/r. \quad (3)$$

A and C are fixed according to the parametrization of this potential for Ca^{2+} ion. Variation of the ion size is done by changing r_0 .

Second model of water is TIP4P/2005 [6]. The ion potential is taken in the form of the Lennard-Jones potential superimposed to Coulomb potential with electronic continuum correction [7]. Variation of the ion size is done by changing σ of the ion Lennard-Jones potential.

Water modelling is performed at $T=300 \text{ K}$ and $\rho = 1 \text{ g/cm}^3$.

All ions in water have charge $+2e$. One ion is added to 1000 water molecules in case of SPC/E water and 343 water molecules in case of TIP4P/2005 water. Langevin thermostat with dumping constant of 15 ps is applied to the system. A time step of numerical integration is 1 fs. Long-range forces are computed by PPPM method. Result is averaged over different initial conditions in addition to time average. Total length of the trajectory is from 15 ns at big ion size to 150 ns at small ion size.

Diffusivity is obtained from the ion mean square displacement, using Einstein relation

$$\langle r^2 \rangle = 6Dt. \quad (4)$$

Dependence of $\langle r^2 \rangle$ on t is averaged over the trajectory. Then D is obtained from the slope of the dependence of $\langle r^2 \rangle$ on t . The results are additionally averaged over the independent trajectories. From 3 to 10 molecular dynamics trajectories are used in case of water. A variation of the average diffusivity is determined from these results. A statistical error for liquid water is shown in figure 2 of the main text. A single trajectory is used for ion in liquid xenon. Additional averaging over independent trajectories is performed for an ion in xenon with $R_{ion} = 1.98 \text{ \AA}$. It is shown that improvement of the accuracy due to the averaging over different trajectories is about 2%.

Diffusivity correction due to small system size [8] is considered together with correction due to incorrect liquid viscosity. The method is the same as used in [8,9] for K^+ ions and RNA. System size correction for ion in water is taken from [8]. Firstly, size correction is applied. Small ion diffusivity is multiplied by $\eta_{model}/\eta_{experiment}$, where η_{model} is liquid viscosity in molecular dynamics and $\eta_{experiment}$ is experimental value of liquid viscosity. Correction for big ions is assumed to be equal to correction for small ions as their solvation shell diffusivity is the same.

Experimental and theoretical values of SPC/E and TIP4P/2005 water viscosity is taken from [10]. Experimental value of liquid xenon viscosity is taken from [11]. Value of viscosity of Lennard-Jones liquid is calculated from the Green–Kubo relation. Moreover, size correction can not affect shape of the dependence of diffusivity on ion radius. It only shifts the entire dependence.

Ion radius is defined as a distance between an ion and xenon atom or oxygen of water molecule.

Ion coordination number is determined as

$$N_c = \sum_{i=1}^{N_{neutral}} \frac{1 - (d/d_0)^{24}}{1 - (d/d_0)^{48}}. \quad (5)$$

Where d is ion-molecule distance, d_0 is a distance from ion to the first minimum of the radial distribution function. This definition of coordination number has a form described in [12, 13]. Free energy as a function of coordination number is determined from histogram of coordination number using a relation

$$F(N_c) = -T \times \ln[P(N_c)], \quad (6)$$

where $P(N_c)$ is number of configurations with coordination number $N_c \pm \Delta N_c$ during the simulation.

Calculations are carried out using Large-scale Atomic/Molecular Massively Parallel Simulator(LAMMPS) [14]. COLVARS module is used to calculate ion coordination number.

Temperature dependence

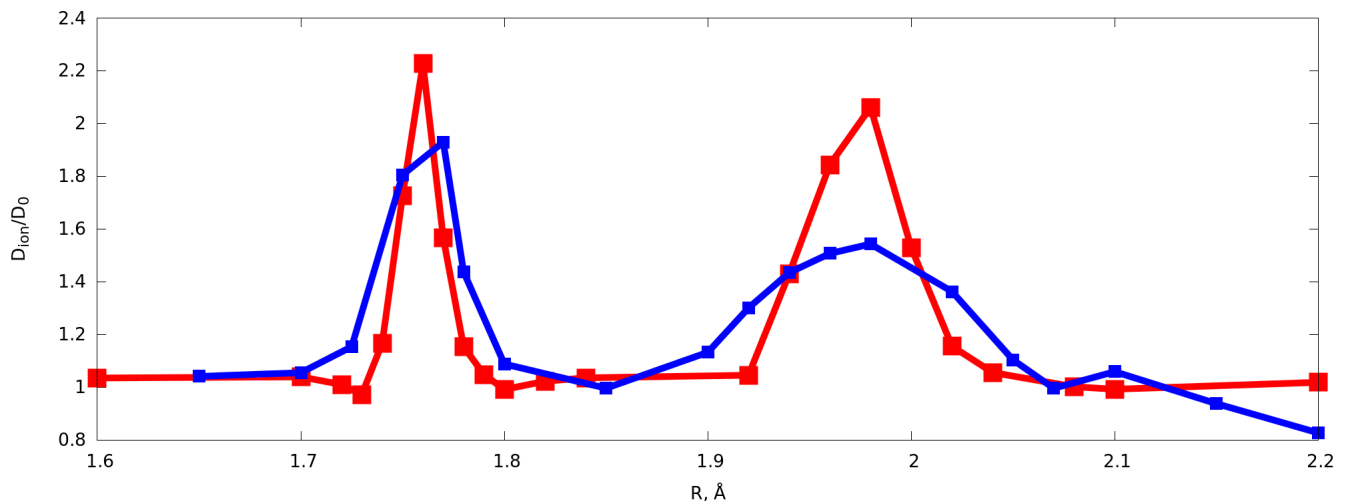


Figure 1: Dependence of the ion diffusivity divided by a diffusivity at small ion size on ion radius in liquid xenon according to molecular dynamics. Red line corresponds to $T=163\text{ K}$, blue line corresponds to $T=310\text{ K}$. Xenon density is $\rho = 3\text{ g/cm}^3$.

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