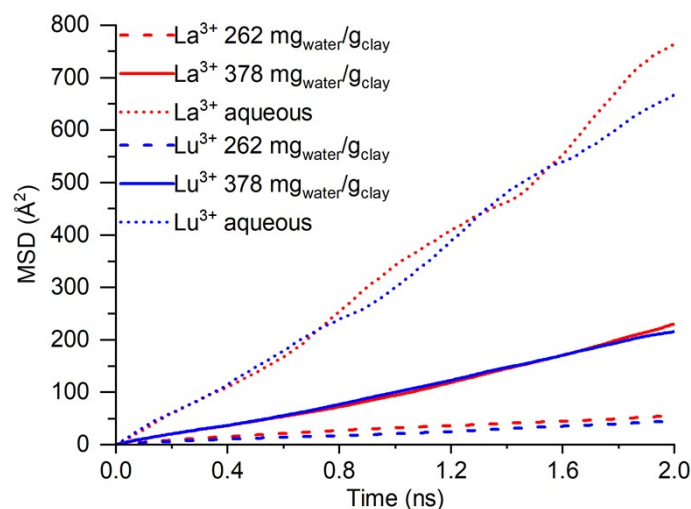




## 8 S1. Mean Square Displacements of $\text{La}^{3+}$ and $\text{Lu}^{3+}$

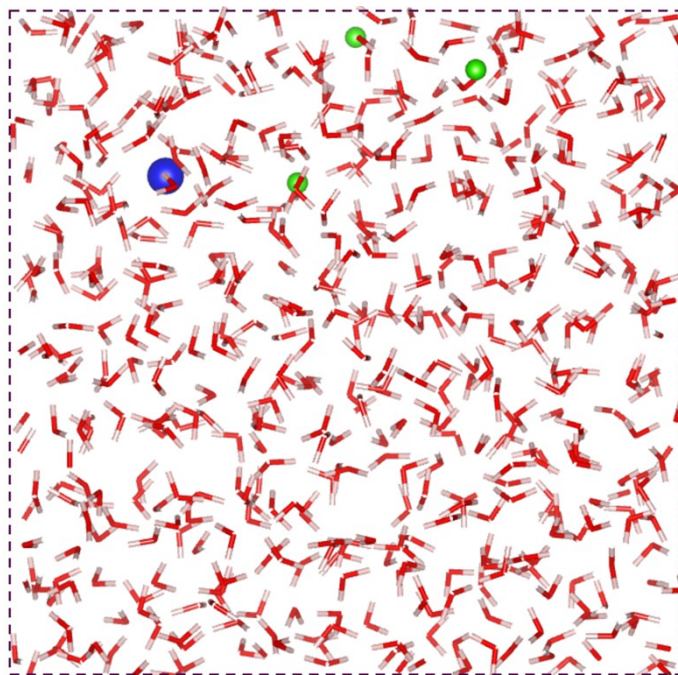


9

10 **FIGURE S1.** 3D Mean square displacements of  $\text{La}^{3+}$  and  $\text{Lu}^{3+}$  in the interlayer spaces  
11 of montmorillonites at 262 mg<sub>water</sub>/g<sub>clay</sub> and 378 mg<sub>water</sub>/g<sub>clay</sub> and in aqueous solutions.

## 12 S2. Simulation Details for $\text{La}^{3+}$ and $\text{Lu}^{3+}$ in Aqueous Solution

13 The aqueous solution contained one  $\text{La}^{3+}/\text{Lu}^{3+}$ , three  $\text{Cl}^-$ , and 512 water molecules  
14 in a cubic box with a side length of 24.7 Å (Fig S2). The density of water is 1 g/cm<sup>3</sup>.  
15 Force field parameters for counter ion  $\text{Cl}^-$  was developed by Joung and Cheatham.<sup>1</sup> The  
16 periodic boundary condition was imposed on three dimensions in all simulations. The  
17 Ewald summation was used to calculate the Coulombic interaction with a precision of  
18  $1.0 \times 10^{-4}$  and a real-space cutoff radius of 10.0 Å. The van der Waals interactions had  
19 a cutoff radius of 10.0 Å. For each simulation, a production run was performed for over  
20 2 ns in NVT (298.15 K). The temperature of the system was controlled by using a Nose-  
21 Hoover chain thermostat. The time step for all simulations was 1.0 fs.



22

23 **FIGURE S2.** Model of La<sup>3+</sup> in aqueous solution. O = red, H = white, Cl<sup>-</sup> = green, and

24 La<sup>3+</sup> = blue.

25

26 **References**

- 27 1. Joung, I. S.; Cheatham III, T. E., Determination of alkali and halide monovalent ion  
28 parameters for use in explicitly solvated biomolecular simulations. *The journal of*  
29 *physical chemistry B* **2008**, *112* (30), 9020-9041.

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