Supplemental Material to "Molecular dynamics study of structural and diffusion properties of dehydrated double layered aluminum and lithium hydroxide"

1. Quantum mechanical calculations.

The QUANTUM ESPRESSO package was used to calculate the electron density. Hereinafter, the latest versions of the programs were used at the time of publication of this article. All files are in the archive **QE_calculations.zip** , including the used pseudopotentials.

The electron density calculation is started by the program **pw.x**. Output of electron density in [.cube] format is performed by the program **pp.x**.

2. Calculation of effective charges.

The calculation of effective charges by the DDEC6 method was performed in the Chargemol program, which can be found at github.com/berquist/chargemol. The [.cube] file of electron density under the name [valence_density.cube] should be placed in the folder with the executable file, after which the file job_control.txt should be filled in. Here it is separately noted that lithium has 3 valence electrons in the used pseudopotentials. All input and output files are in the archive **Chargmol_calculations.zip**.

The same file [valence_density.cube] was also placed next to the executable file of the program for calculating Bader charges, see theory.cm.utexas.edu/henkelman/code/bader/.
All output files are in the archive **bader_calculations.zip**.

3. Molecular dynamics calculations.

The LAMMPS files for analyzing the influence of the angle interaction on the model are given in the archive **angle_calculations.zip**. By visualizing [dump.LDH], one can verify the instability of the structure at high temperatures. Further dump files will not be attached due to their large size (about a gigabyte per calculation).

The files of molecular dynamics calculations with Bader charges are given in the archive **bader_md_calculations.zip**.

Files of structural property calculations for the final model with DDEC6 are in the archive **md_structure.zip**. Also in the archive are scripts for analyzing dump files: [avg_geom.ipynb] for averaging cell parameters over time, [dens_Oz.ipynb] for plotting particle distribution density along the lamellar layer, [RDF.ipynb] for plotting radial distribution functions.

The files for analyzing the equilibrium yields using different ensembles are in the archive **RMSD_calculations.zip**. The script [RMSE.ipynb] for analyzing dump files and plotting graphs is also attached.

4. Diffusion calculations.

Lammps scripts for analysis of interlamellar lithium diffusion and processing script [diffusion_calc.ipynb] on dump file are attached in the archive **main_diffusion.zip**. In the processing script it is necessary to specify the name of dump file and write the necessary index of particle in the code, it will plot all coordinates from time on one graph, after that it will calculate the coefficient of two-dimensional diffusion. This archive also contains files for the enlarged model.

The files corresponding to the calculation of the effect of perturbation of effective charges are in the archive **perturbation_diffusion.zip**.