

Description of Additional Supplementary Files

Supplementary Data 1. Dissolution energy of 4Al: Al-0H₂O.xyz, Al-1H₂O.xyz, Al-2H₂O.xyz, Al-3H₂O.xyz, Al-4H₂O.xyz.

Supplementary Data 2. Dissolution energy of DCE41: Al-0H₂O-Zn-0H₂O.xyz, Al-1H₂O-Zn-0H₂O.xyz, Al-1H₂O-Zn-1H₂O.xyz, Al-2H₂O-Zn-1H₂O.xyz, Al-2H₂O-Zn-2H₂O.xyz, Al-2H₂O-Zn-3H₂O.xyz, Al-3H₂O-Zn-3H₂O.xyz, Al-4H₂O-Zn-3H₂O.xyz, Al-4H₂O-Zn-4H₂O.xyz, Al-4H₂O-Zn-5H₂O.xyz.

Supplementary Data 3. Binding energy: Al-H₂O.xyz, Ca-H₂O.xyz, Li-H₂O.xyz, Mg-H₂O.xyz, Na-H₂O.xyz, Zn-H₂O.xyz.

Supplementary Data 4. Solvation energy: Al-6H₂O.mol2, Ca-8H₂O.mol2, Li-4H₂O.mol2, Mg-6H₂O.mol2, Na-6H₂O.mol2, Zn-6H₂O.mol2.

Supplementary Data 5. Hirshfeld charge distributions: Al-H₂O.mol2, Ca-H₂O.mol2, Li-H₂O.mol2, Mg-H₂O.mol2, Na-H₂O.mol2, Zn-H₂O.

Supplementary Data 6. MD of H₂O : Initial structure: H₂O.gro; Balanced structure: H₂O.gro.

Supplementary Data 7. MD of different ions (298.15 K): Initial structure: Al.gro, Ca²⁺.gro, Li.gro, Mg.gro, Na.gro, Zn.gro; Balanced structure: Al.gro, Ca.gro, Li⁺.gro, Mg.gro, Na.gro, Zn.gro.

Supplementary Data 8. MD of different ions (273.15 K): Initial structure: Al.gro, Ca.gro, Li.gro, Mg.gro, Na.gro, Zn.gro; Balanced structure: Al.gro, Ca.gro, Li.gro, Mg.gro, Na.gro, Zn.gro.

Supplementary Data 9. MD of different ions (253.15 K): Initial structure: Al.gro, Ca.gro, Li.gro, Mg.gro, Na.gro, Zn.gro; Balanced structure: Al.gro, Ca.gro, Li.gro, Mg.gro, Na.gro, Zn.gro.

Supplementary Data 10. MD of different concentrations of Al: Initial structure: 1Al.gro, 2Al.gro, 3Al.gro, 4Al.gro, 5Al.gro, 5.3Al.gro. Balanced structure: 1Al.gro, 2Al.gro, 3Al.gro, 4Al.gro, 5Al.gro, 5.3Al.gro.

Supplementary Data 11. MD of DCE41: Initial structure: DCE41.gro; Balanced structure: DCE41.gro.

Supplementary Data 12. MD of 1Zn: Initial structure: 1Zn.gro; Balanced structure: 1Zn.gro.