Supporting Information for

Interfacial Insights for Divergent Dendrite Formation Mechanisms in Lithium and Magnesium Anodes

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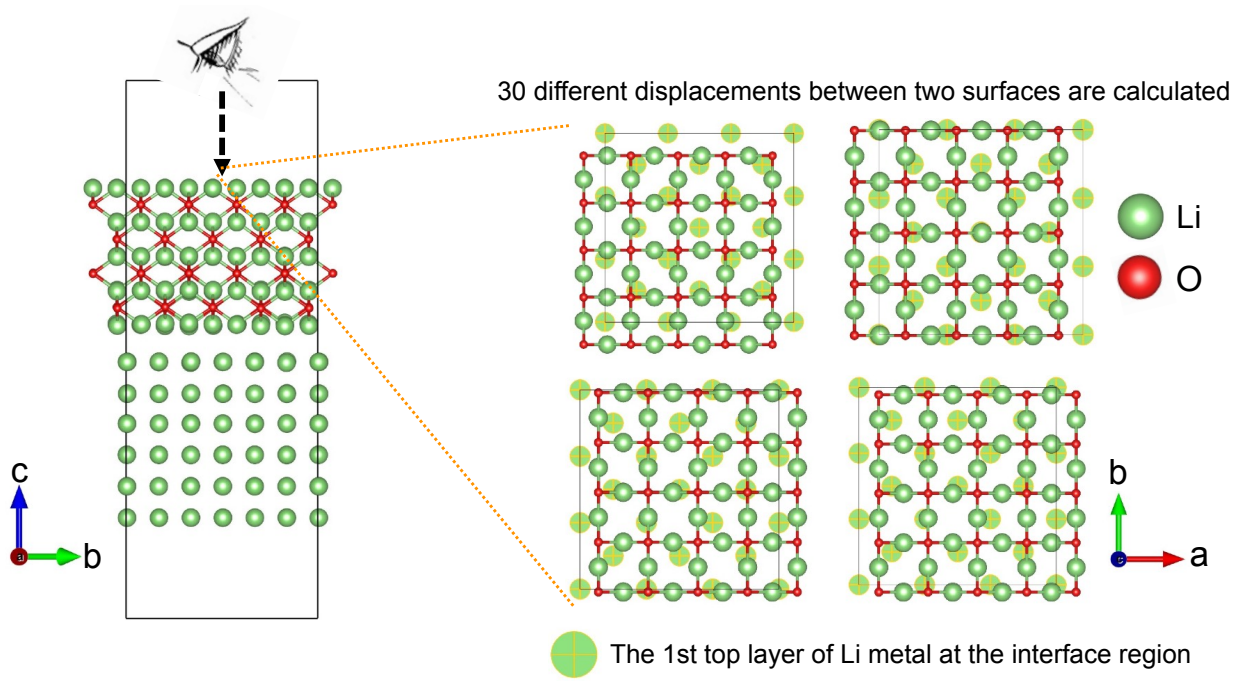

Figure S1. The schematic of the displacement between two surfaces in a heterogeneous interface model.

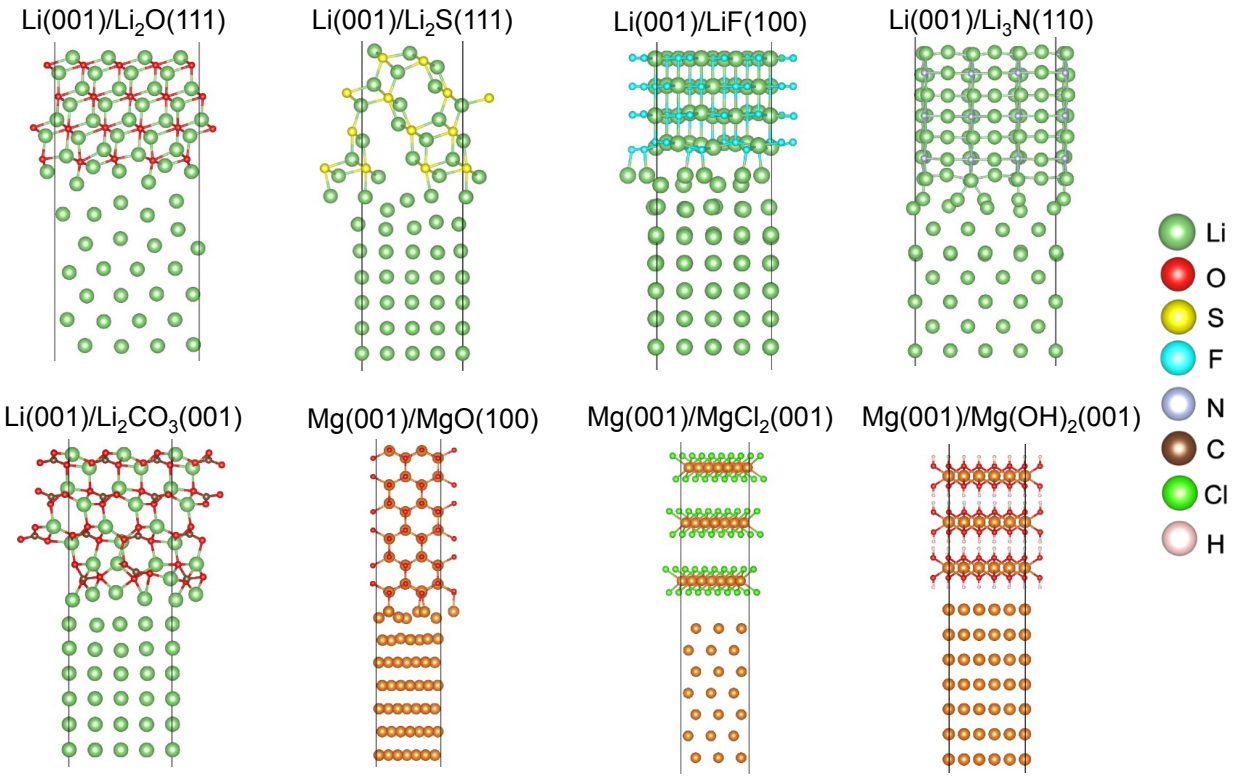

Figure S2. Density Functional Theory (DFT)-optimized interface structures, which are constructed using surfaces with the lowest surface energy.

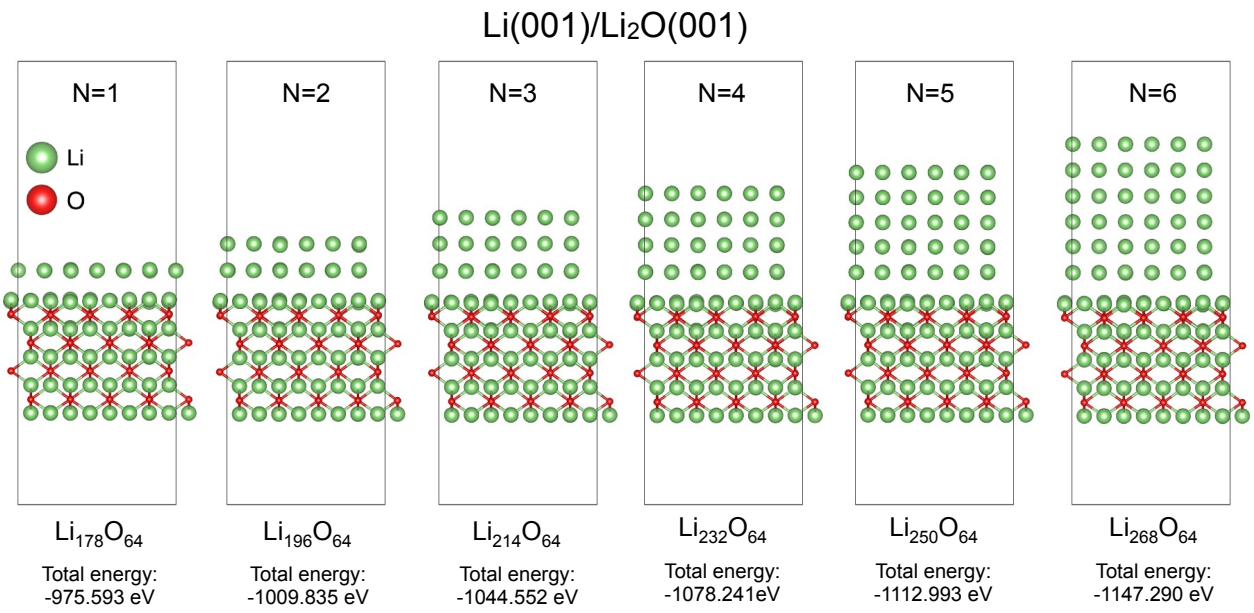

Figure S3. Layer-by-layer deposition of Li(001) atoms onto Li_2O(001) surfaces to compute the plating energy.

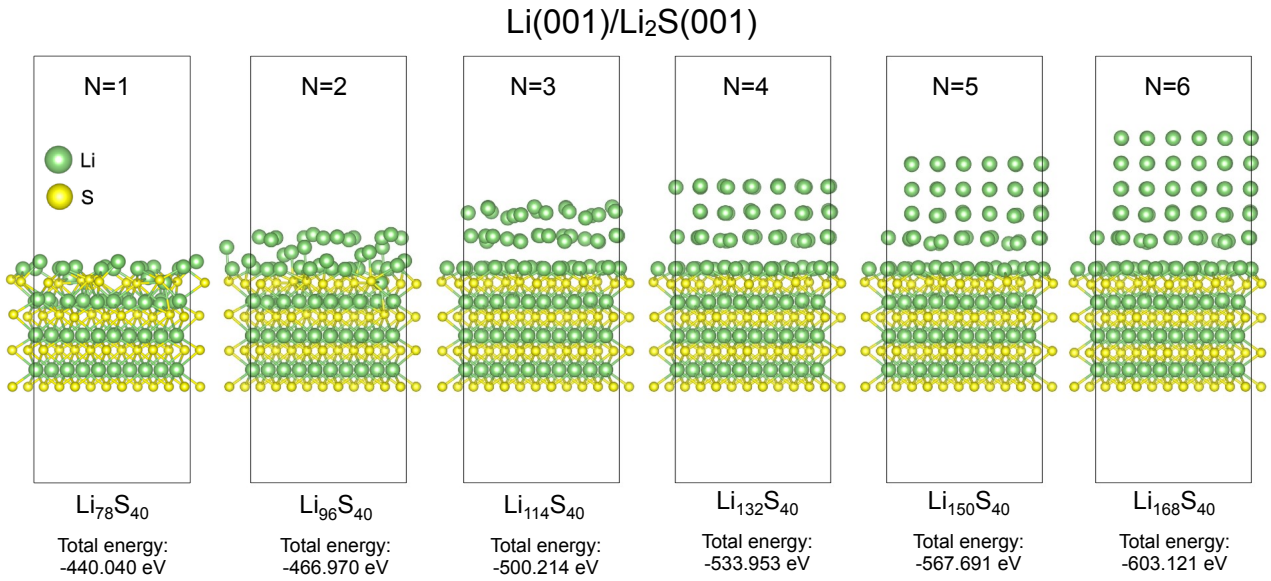

Figure S4. Layer-by-layer deposition of Li(001) atoms onto Li_2S(001) surfaces to compute the plating energy.

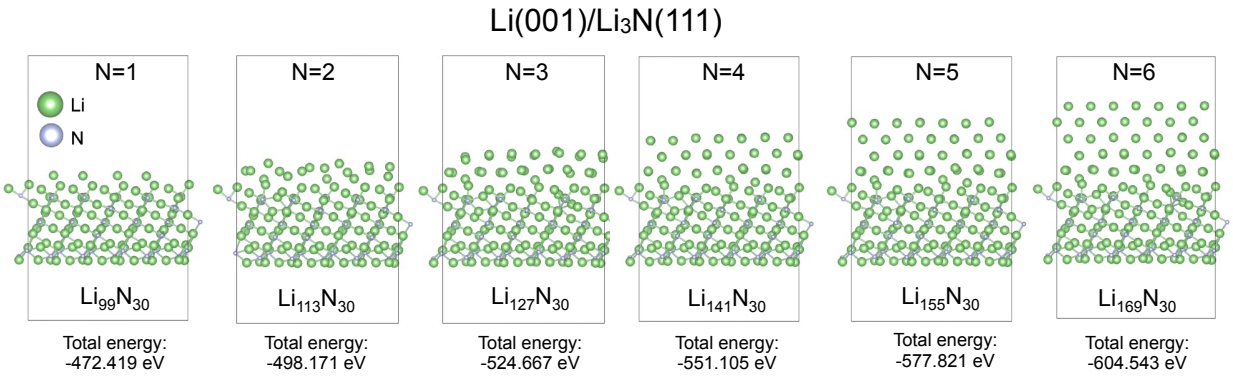

Figure S5. Layer-by-layer deposition of Li(001) atoms onto Li_3N(111) surfaces to compute the plating energy.

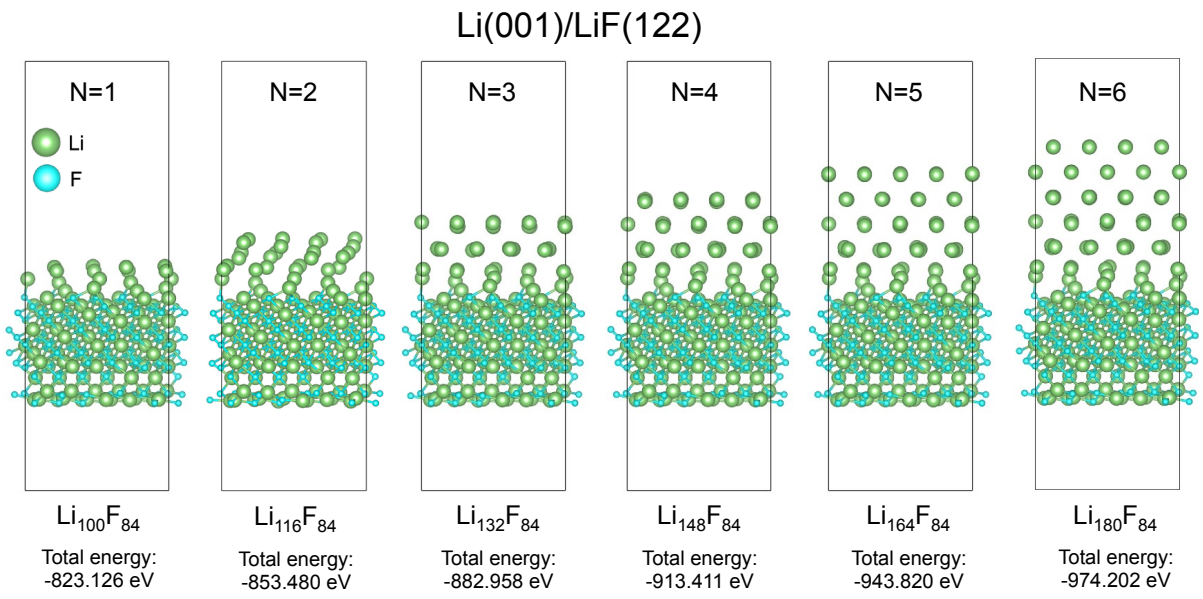

Figure S6. Layer-by-layer deposition of Li(001) atoms onto LiF(122) surfaces to compute the plating energy.

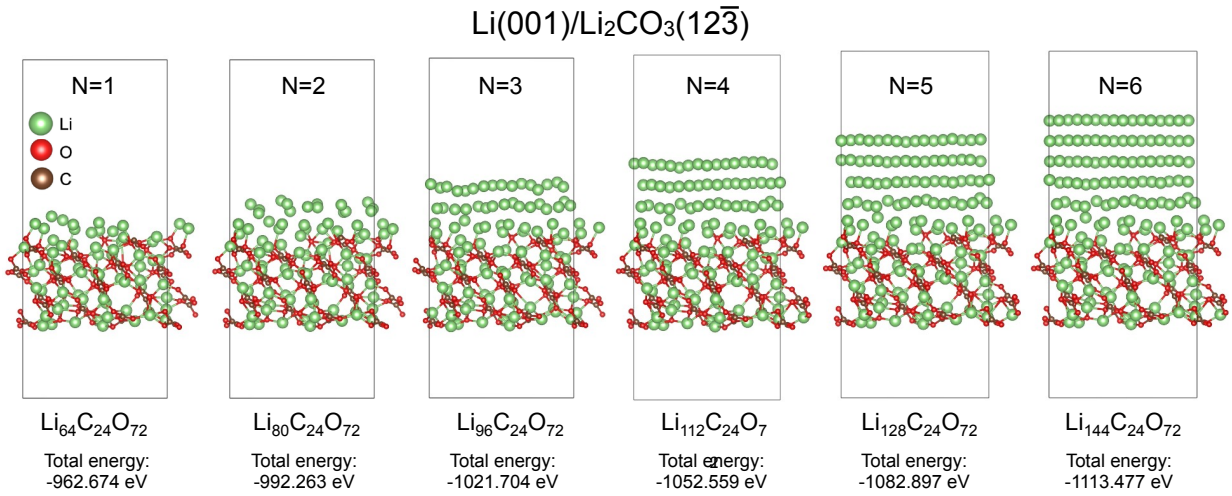

Figure S7. Layer-by-layer deposition of Li(001) atoms onto $Li_2CO_3(12\bar{3})$ surfaces to compute the plating energy.

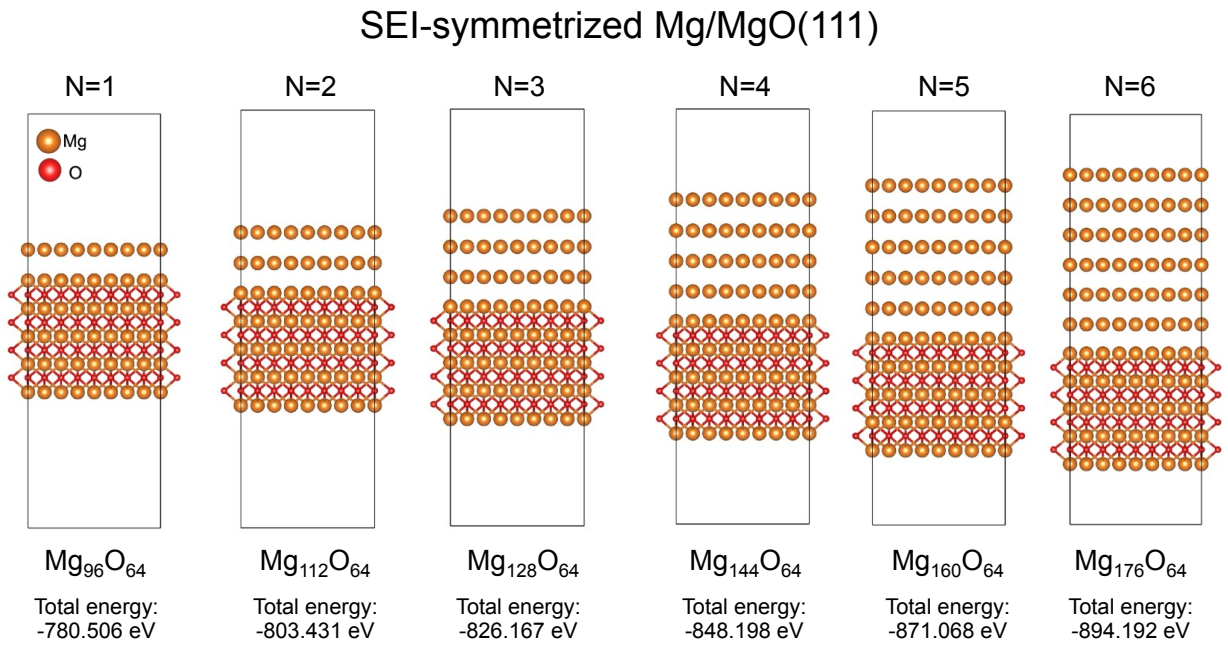

Figure S8. Layer-by-layer deposition of Solid Electrolyte Interphase (SEI)-symmetrized Mg atoms onto MgO(111) surfaces to compute the plating energy.

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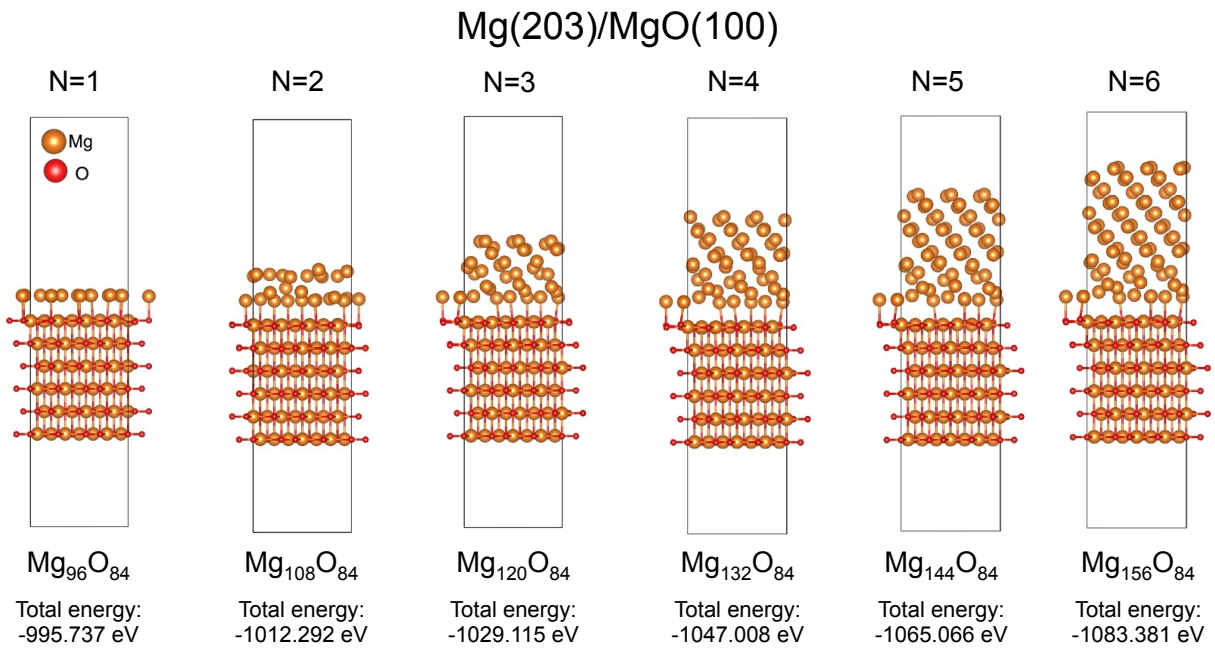

Figure S9. Layer-by-layer deposition of Mg(203) atoms onto MgO(100) surfaces to compute the plating energy.

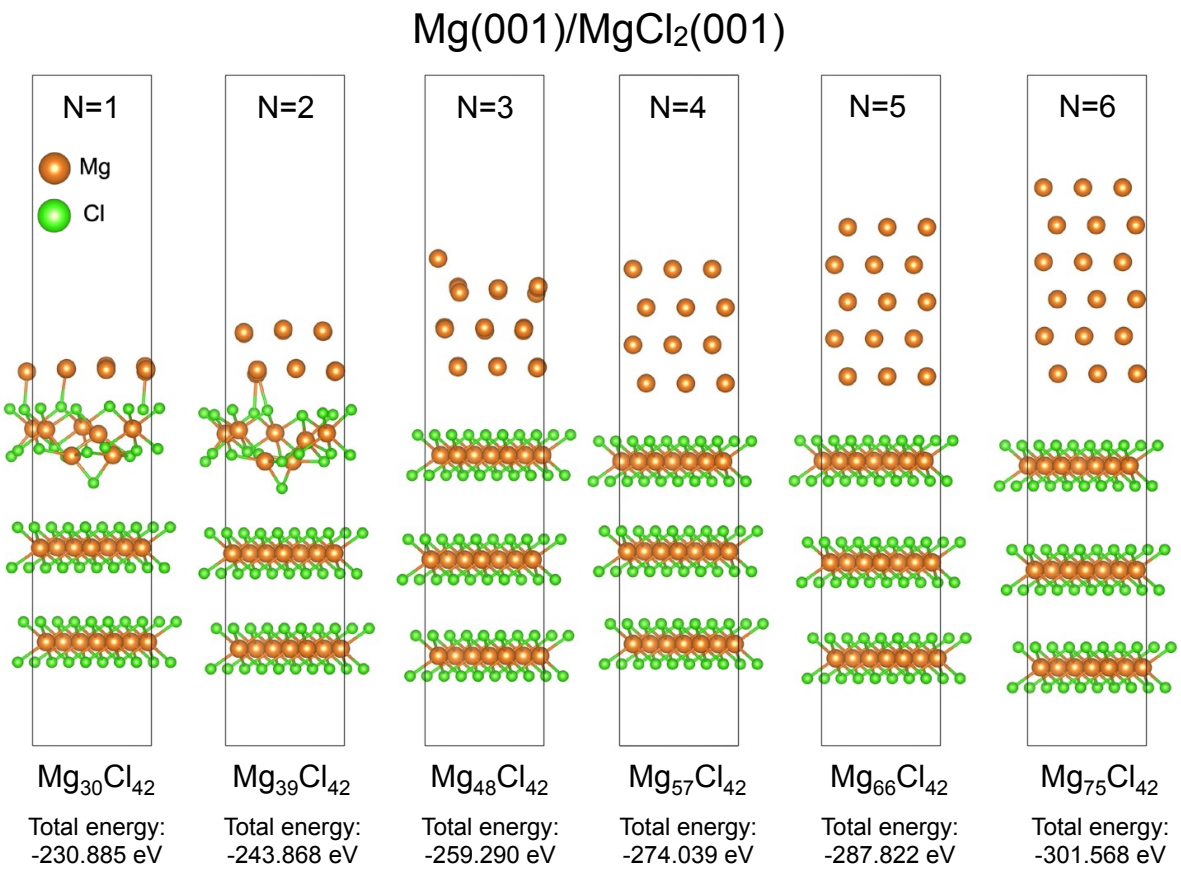

Figure S10. Layer-by-layer deposition of Mg(001) atoms onto $MgCl_2$(001) surfaces to compute the plating energy.

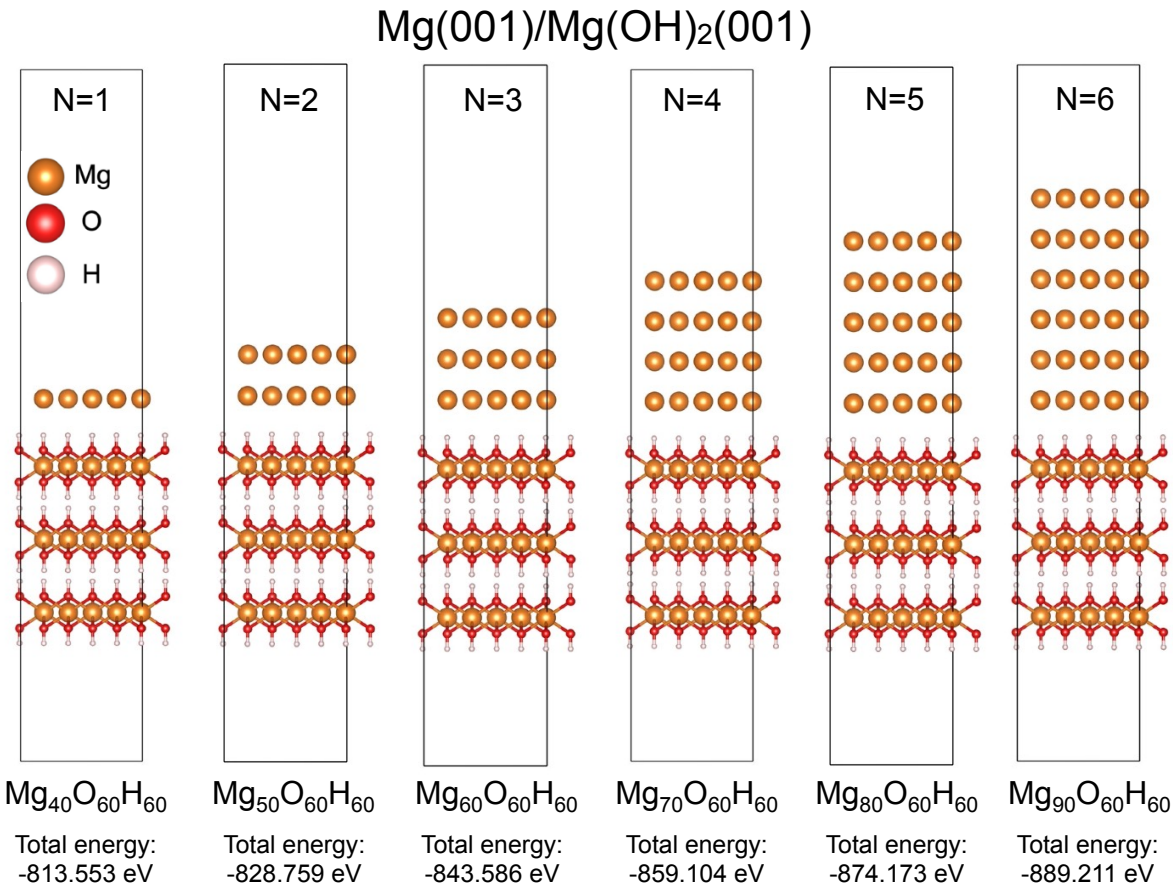

Figure S11. Layer-by-layer deposition of Mg(001) atoms onto $Mg(OH)_2(001)$ surfaces to compute the plating energy.

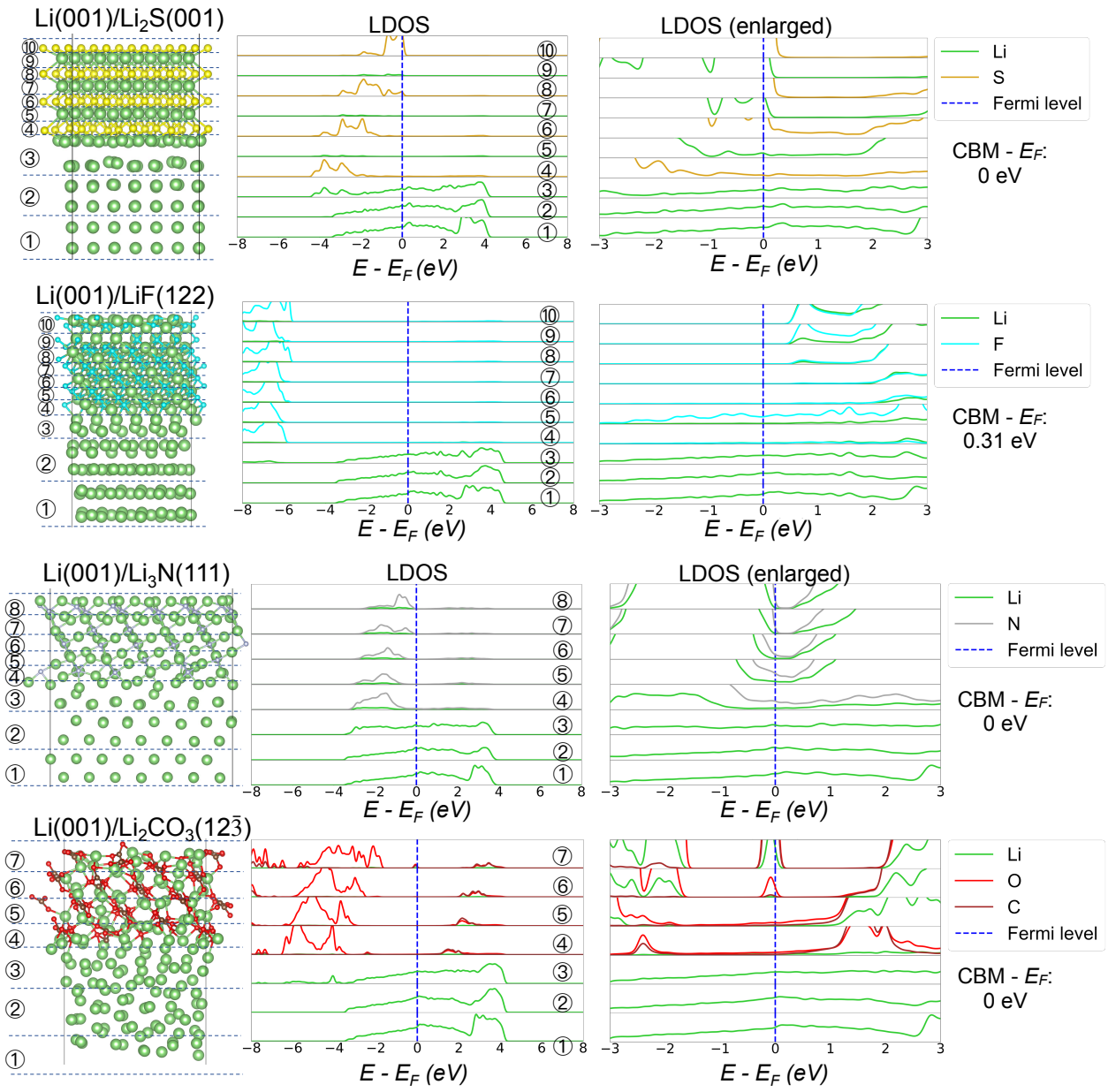

Figure S12. Layer-by-layer Local Density of States (LDOS) calculated for heterogeneous interface structures between Li-SEI surfaces and Li(001) anode surface. The atomic structures are aligned with LDOS to depict the corresponding layer LDOS. Each layer in the interface structure is numbered for reference to the layered LDOS. Energy levels (E) are referenced to zero at the Fermi level (E_F). Enlarged LDOS, with a shorter energy range and reduced intensity range, is provided for enhanced visualization of electronic states around the Fermi level. The difference between the Fermi level and the conduction band minimum (CBM) in the SEI-region (CBM – E_F) is also provided.

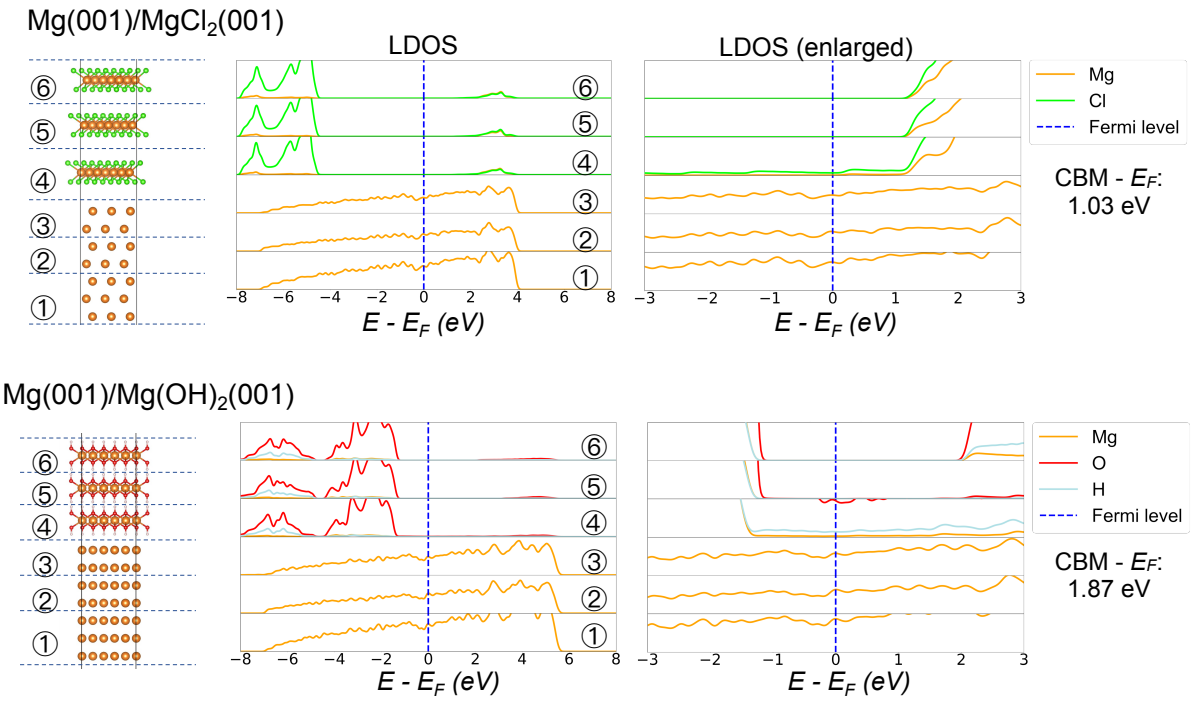

Figure S13. Layer-by-layer LDOS calculated for heterogeneous interface structures between Mg-SEI surfaces and Mg(001) anode surface. The atomic structures are aligned with LDOS to depict the corresponding layer LDOS. Each layer in the interface structure is numbered for reference to the layered LDOS. Energy levels (E) are referenced to zero at the Fermi level (E_F). Enlarged LDOS, with a shorter energy range and reduced intensity range, is provided for enhanced visualization of electronic states around the Fermi level. The difference between the Fermi level and the conduction band minimum (CBM) in the SEI-region (CBM – E_F) is also provided.