Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Understanding the Molecular Mechanism of Lithium Deposition for Practical High-Energy Lithium-Metal Batteries

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Supporting Information

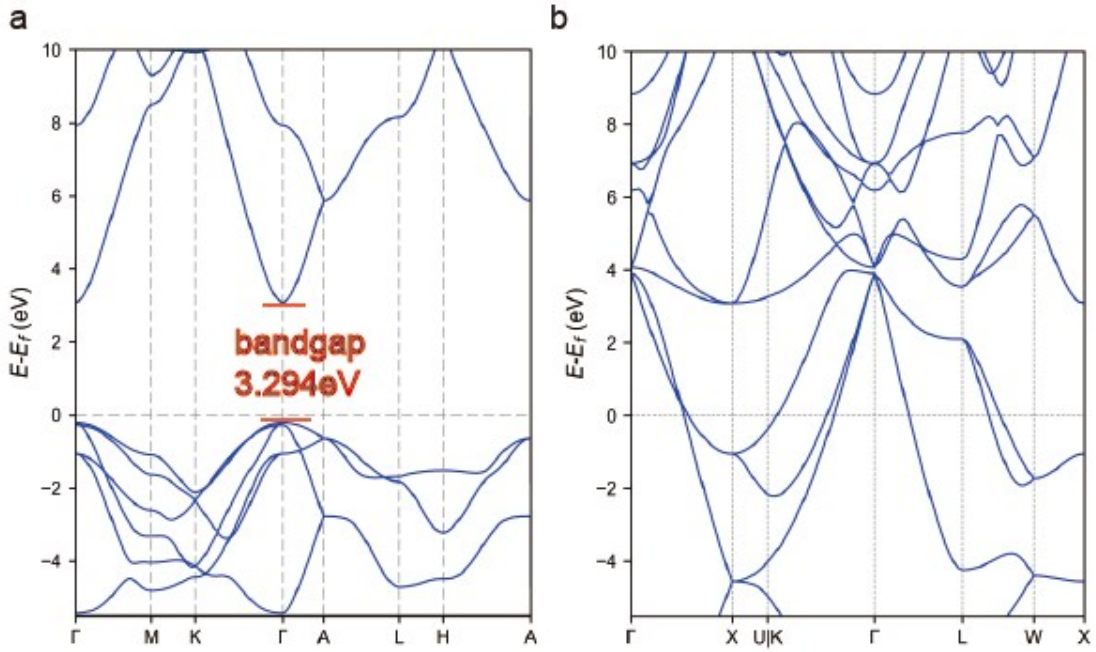

Figure S1. Band structures of (a) ZnO, (b) LiZn. Fermi levels have been set to zero. Bandgap of ZnO was labeled.

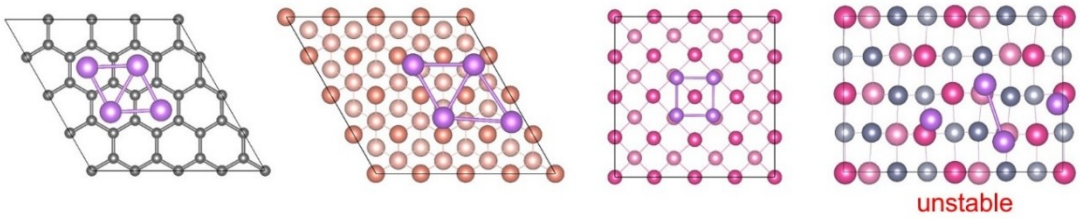

Figure S2. The optimized Li tetramer configurations on (a) the graphene, (b) the Cu(111) surface, (c) the Li(001) surface, and (d) the LiZn(110) surface. The tetramer on LiZn(110) surface is not stable due to mismatched lattices of Li cluster and LiZn.

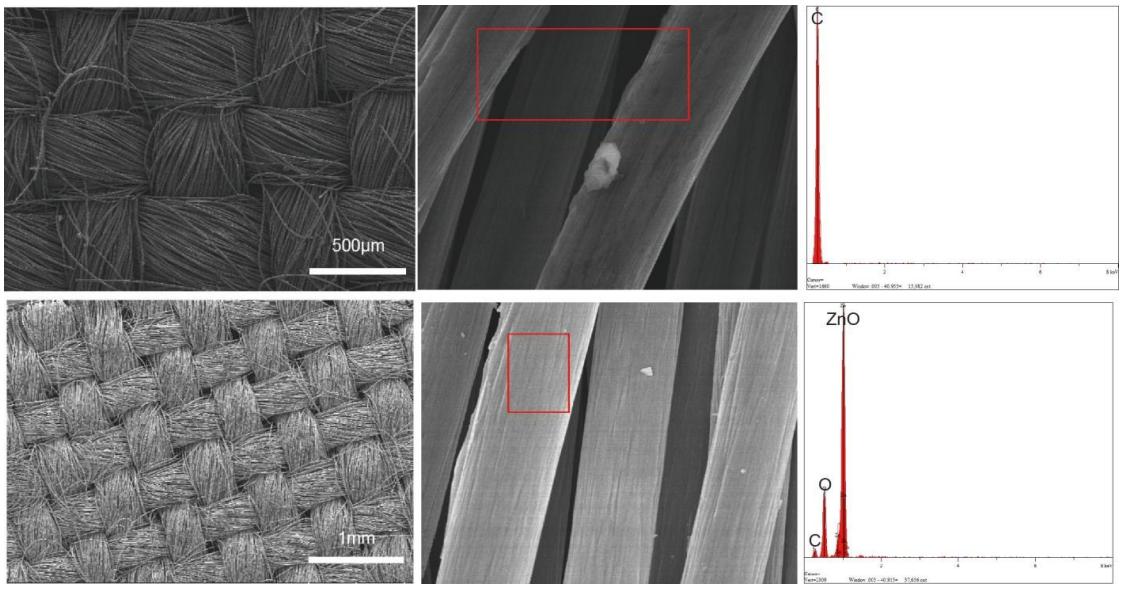

Figure S3. The SEM images and energy dispersive X-ray spectroscopy (EDX) of CF (upper) and CF@ZnO (lower).

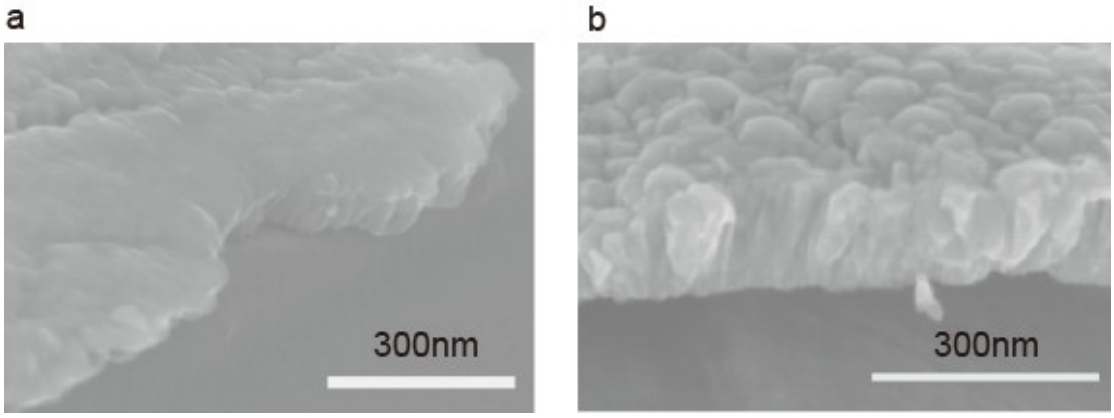

Figure S4. The morphologies of ZnO coating on (a) Cu foiland (b)CF.

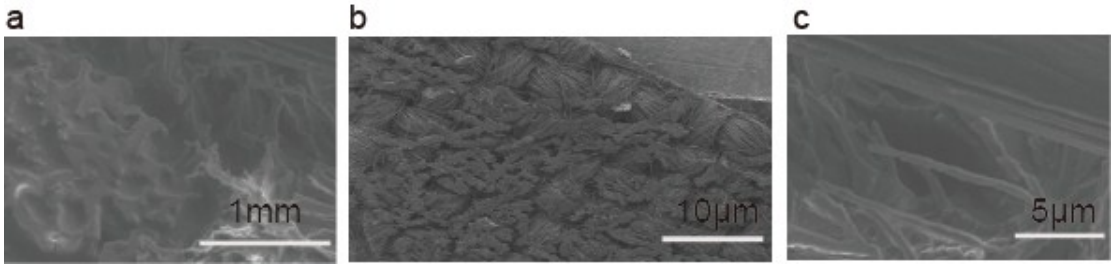

Figure S5. The morphology of CF after Li plating for 1 hour.

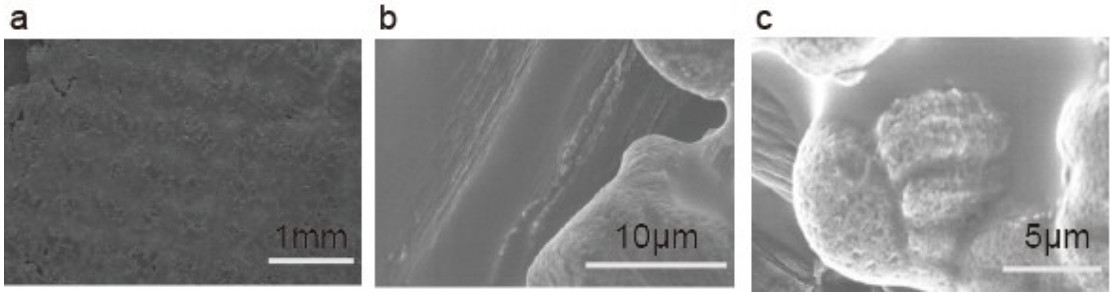

Figure S6. The morphology of CF after Li plating for 3 hours.

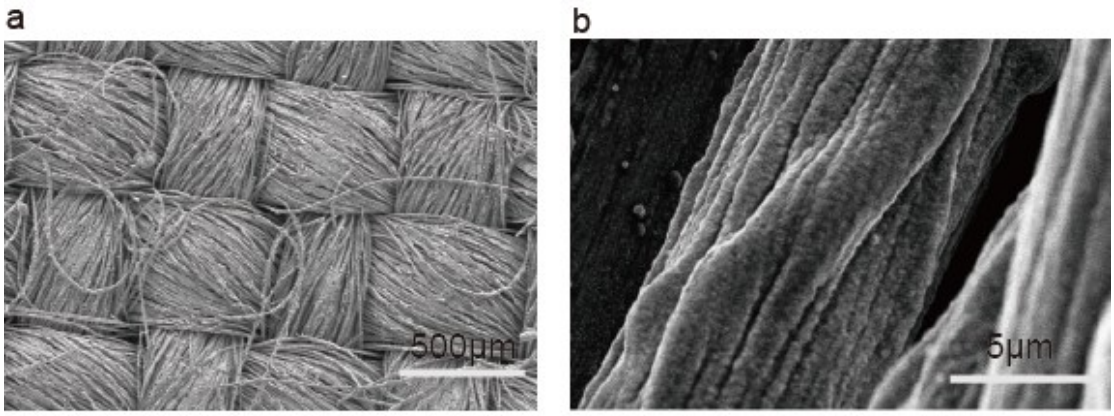

Figure S7. The morphology of CF@ZnO after Li plating for 1 hour.

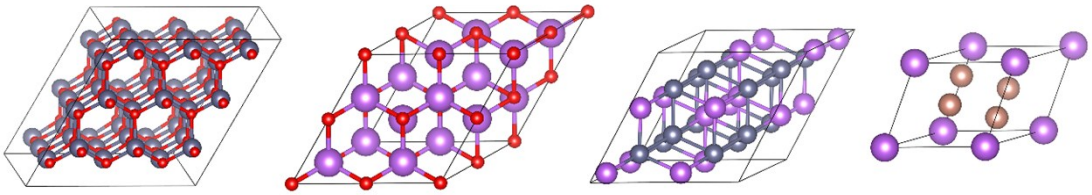

Figure S8. Structures of ZnO, Li_2O, LiZn, and $LiCu_3$ after geometric optimization.

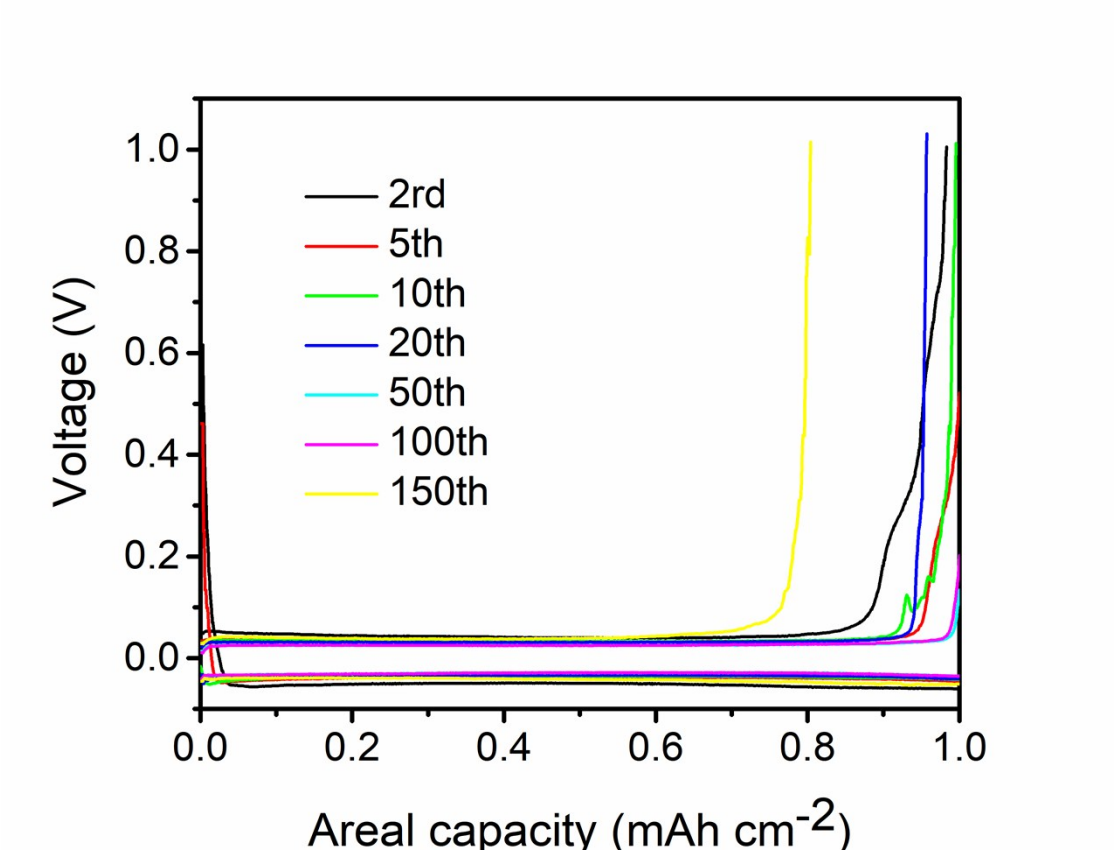

Figure S9. Voltage profiles of Li plating/stripping on ZnO@Cu (40mins) with areal capacity of 1.0 mAh cm^{-2} at current density of 1 mA cm^{-2} at the 2rd, 5th, 10th. 50th, 100th and 150th cycles.

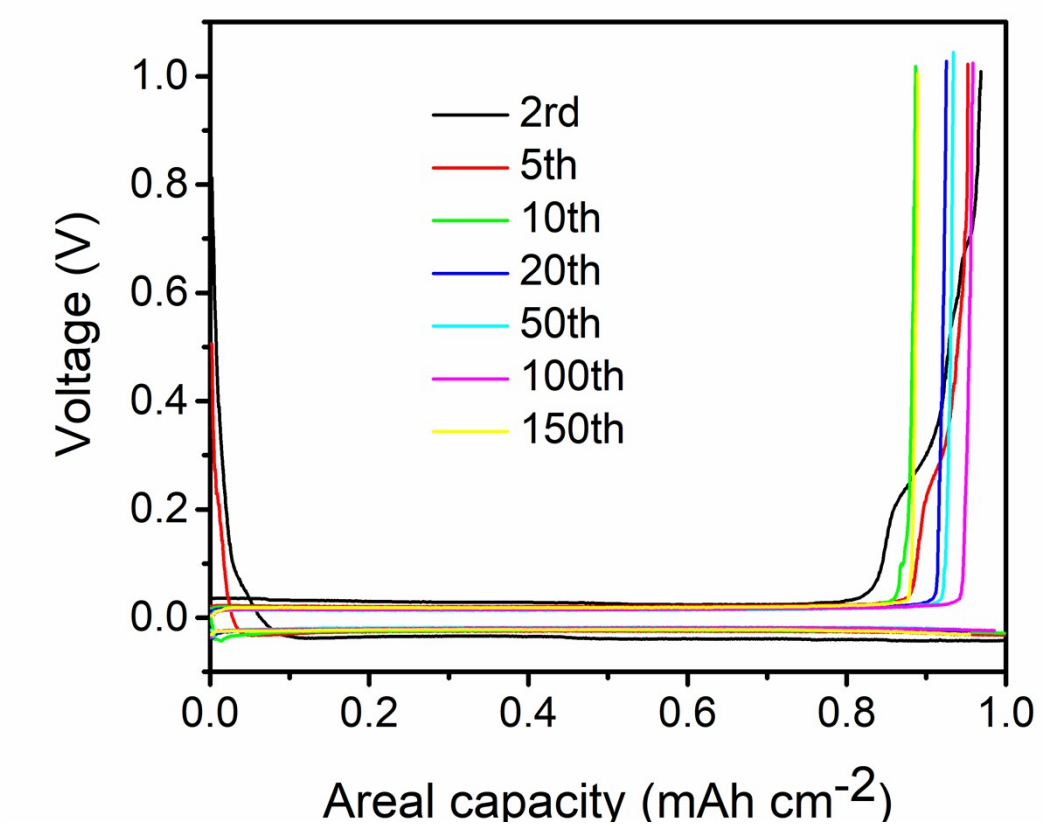

Figure S10. Voltage profiles of Li plating/stripping on ZnO@Cu (150mins) with areal capacity of 1.0 mAh cm^{-2} at current density of 1 mA cm^{-2} at the 2rd, 5th, 10th. 50th, 100th, and 150th cycles.

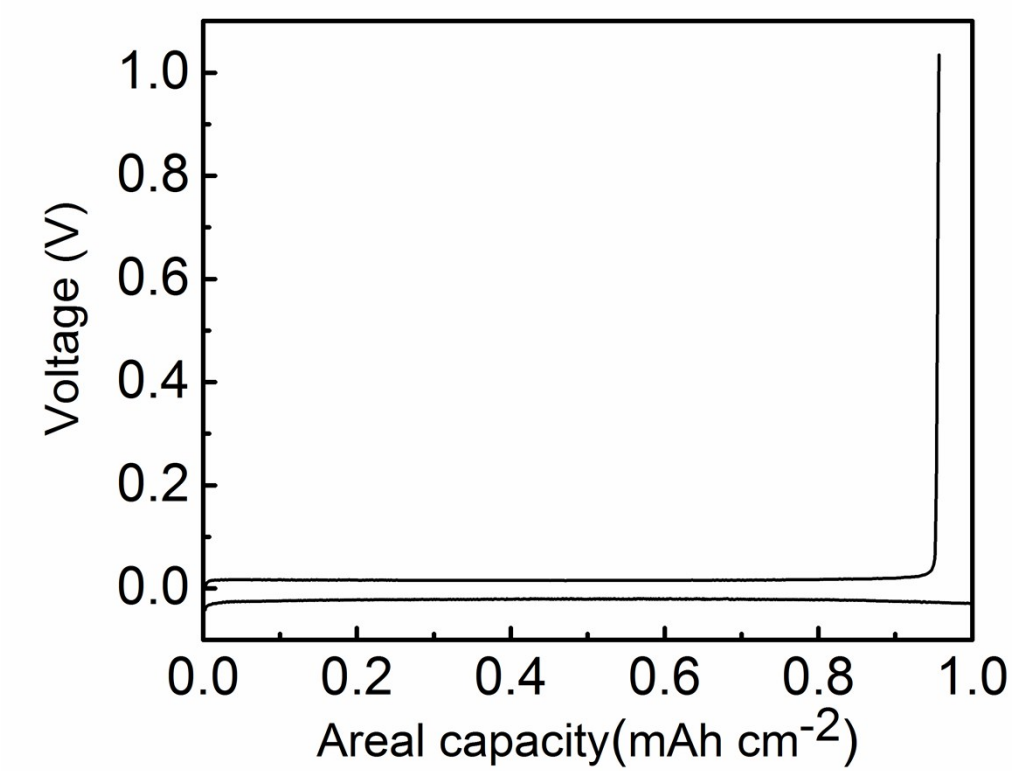

Figure S11. Voltage profiles of initial Li plating/stripping on Cu foil with areal capacity of 1.0 mAh cm^{-2} at a current density of 1 mA cm^{-2}.

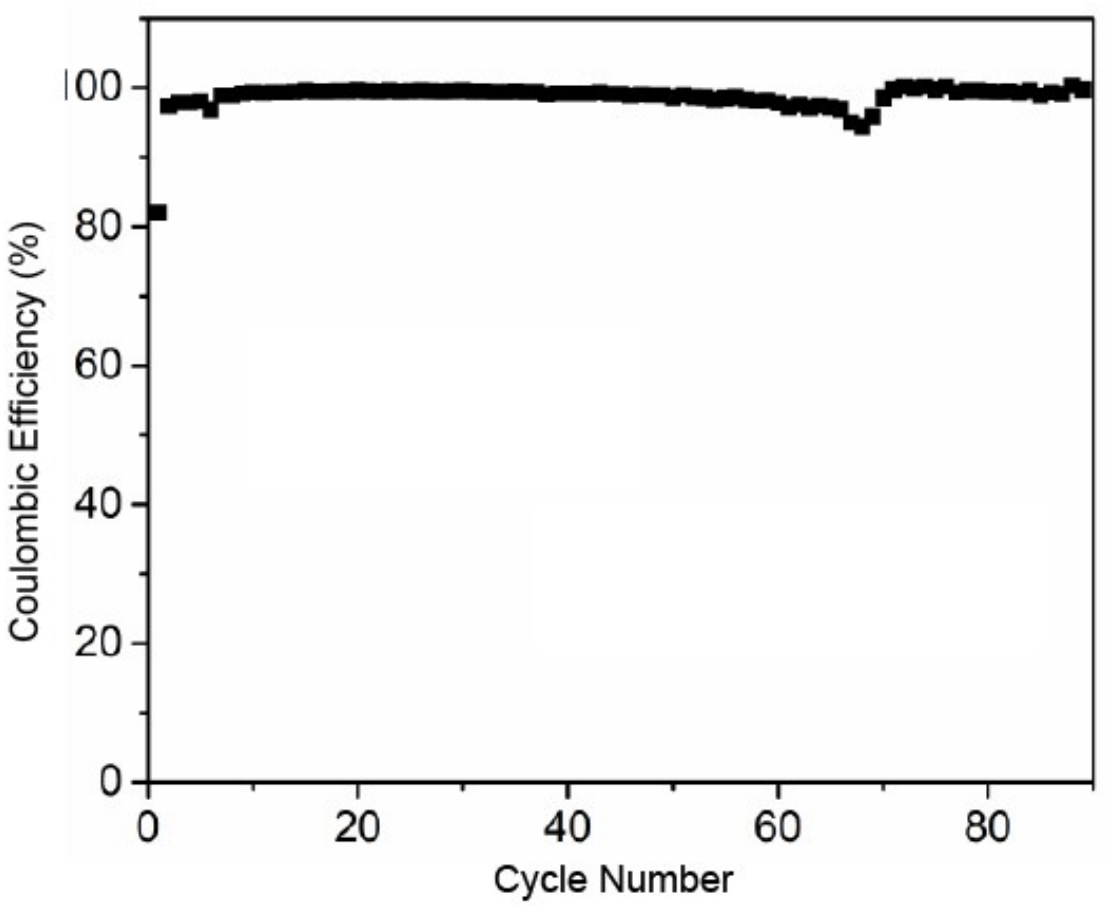

Figure S12. Coulombic Efficiency of cells with ZnO@CF (200mins) at 0.5 mA cm^{-2} (8.0 mAh cm^{-2}).