Supporting Information

Building multifunctional Cu_2Se@biomass carbon composite interfacial layer on zinc anode towards stable aqueous zinc-ion batteries

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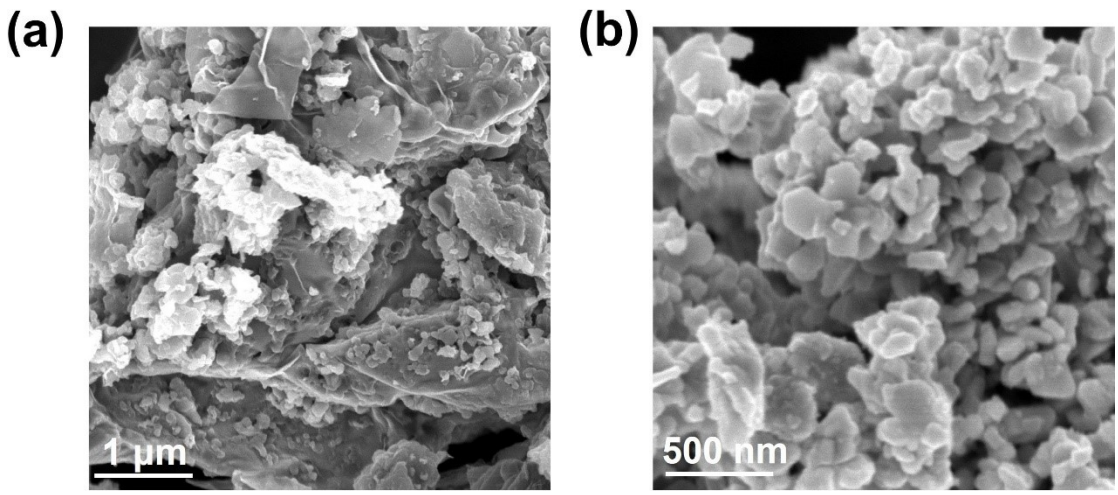

Figure S1. SEM images of (a) Cu_2Se@BC composite and (b) Cu_2Se nanoblock.

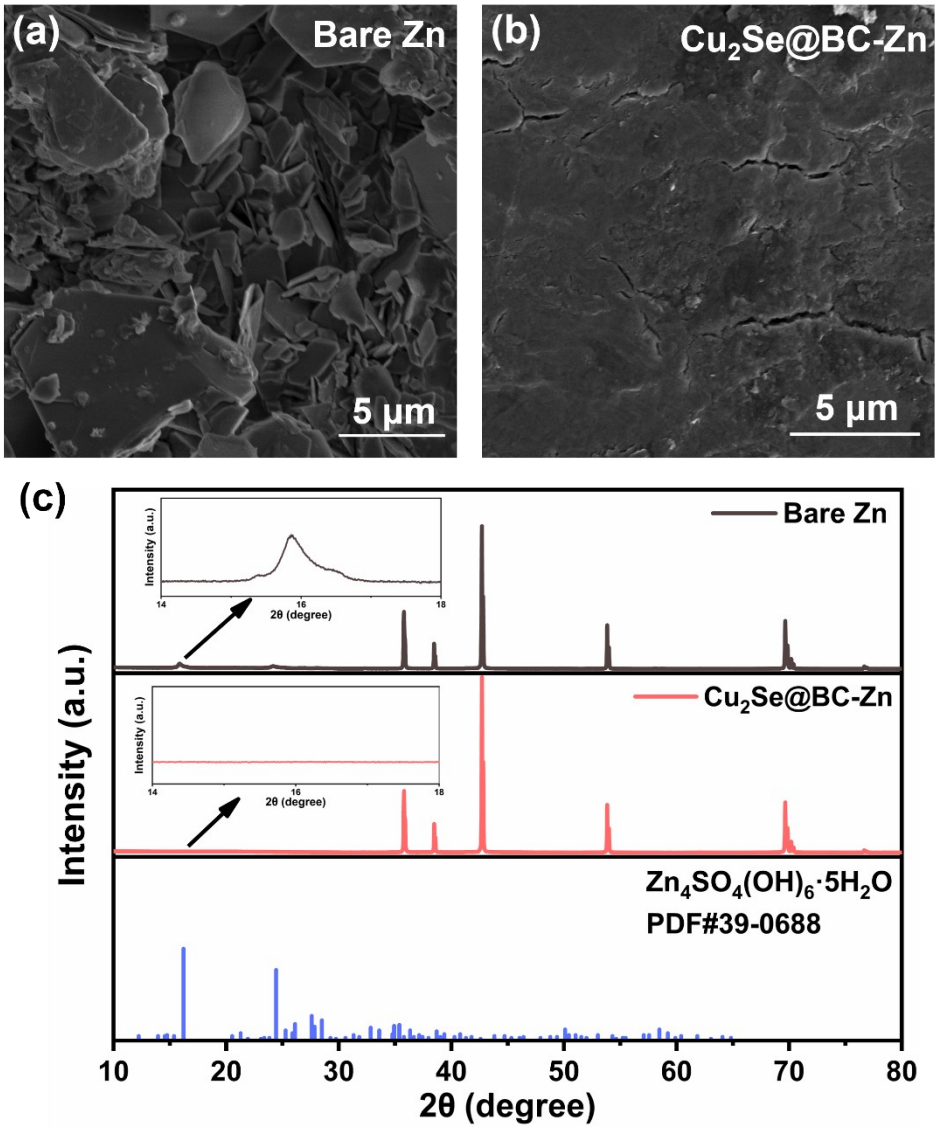

Figure S2. SEM images of (a) bare Zn and (b) Cu_2Se@BC−Zn anode and (c) XRD patterns after soaking in electrolyte for 3 days.

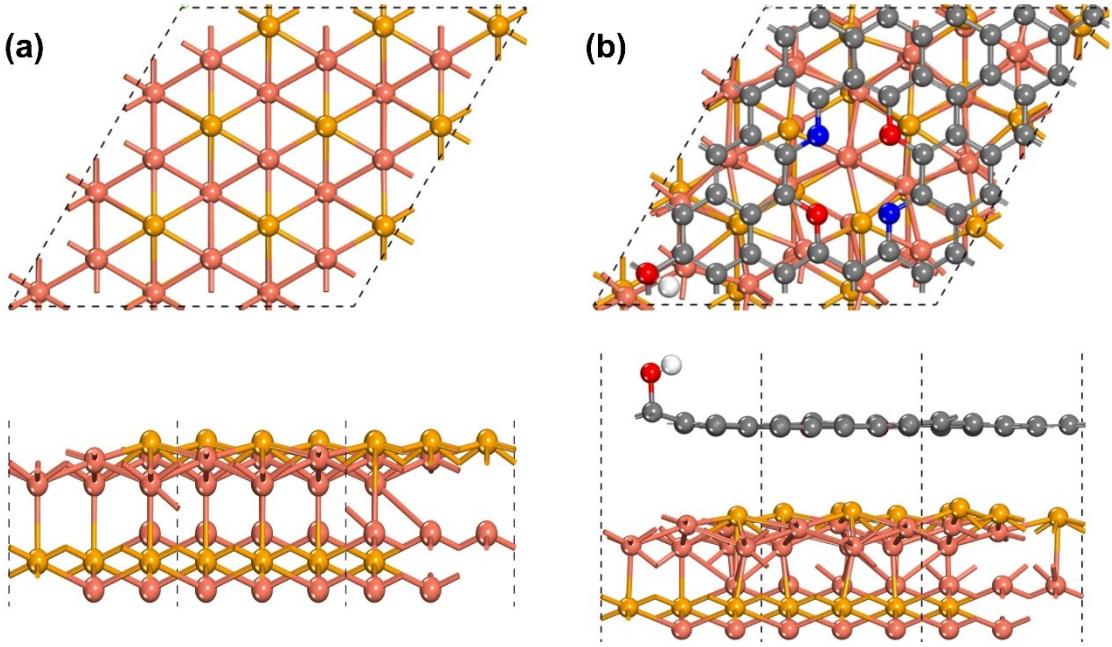

Figure S3. The top (up) and side (down) view of optimized configurations of the (a) Cu_2Se (111) surface and (b) Cu_2Se@BC interface. Amber, coralito, red, blue, white, and blue gray ball marks Se, Cu, O, N, and H atom, respectively.

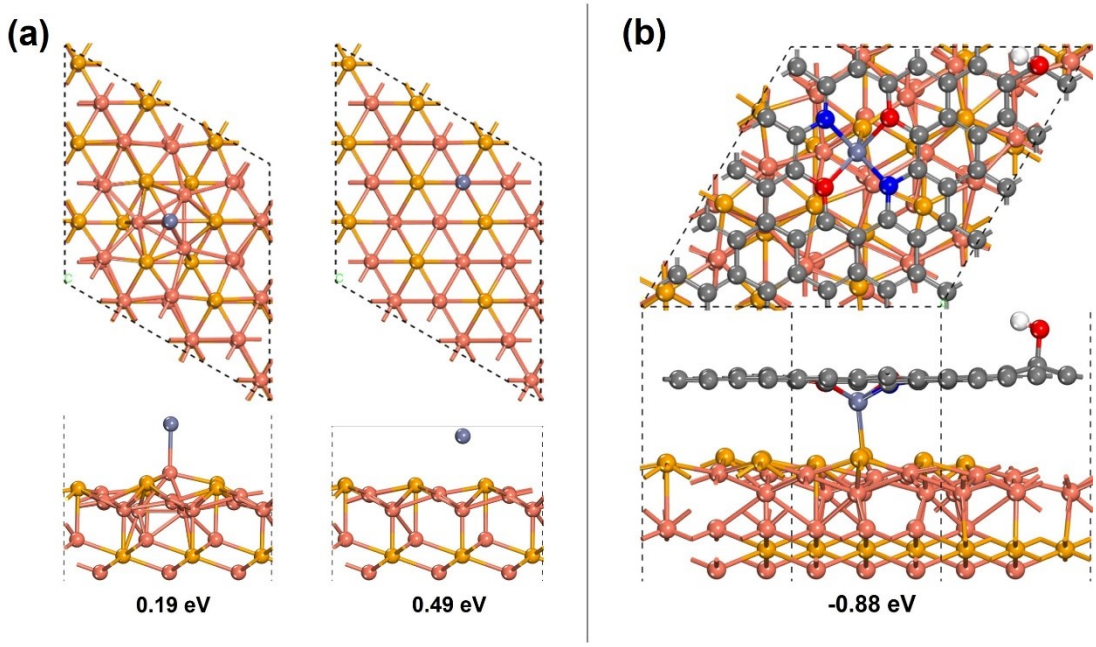

Figure S4. The top (up) and side (down) view of optimized adsorption configuration of Zn atom on (a) the Cu_2Se (111) surface and (b) the interface of Cu_2Se@BC. Amber, coralito, red, blue, white, and blue gray ball marks Se, Cu, O, N, H, and Zn atom, respectively.

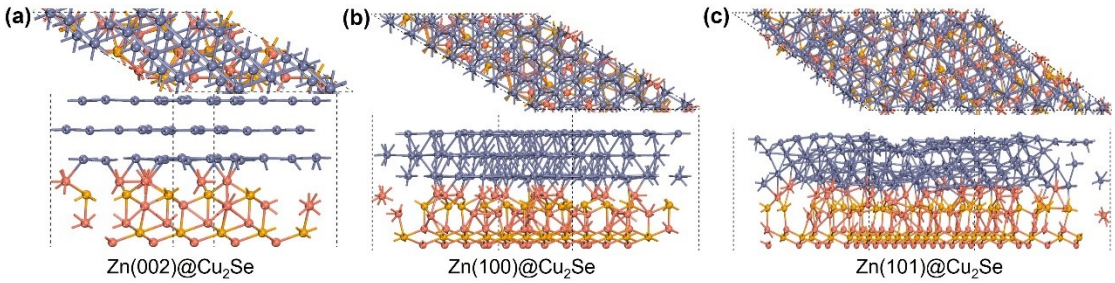

Figure S5. The top (up) and side (down) view of optimized interface configuration of the (a) Zn(002)@Cu_2Se, (b) Zn(100)@Cu_2Se, (c) Zn(101)@Cu_2Se interface. Amber, coralito, and blue gray ball marks Se, Cu, and Zn atom, respectively.

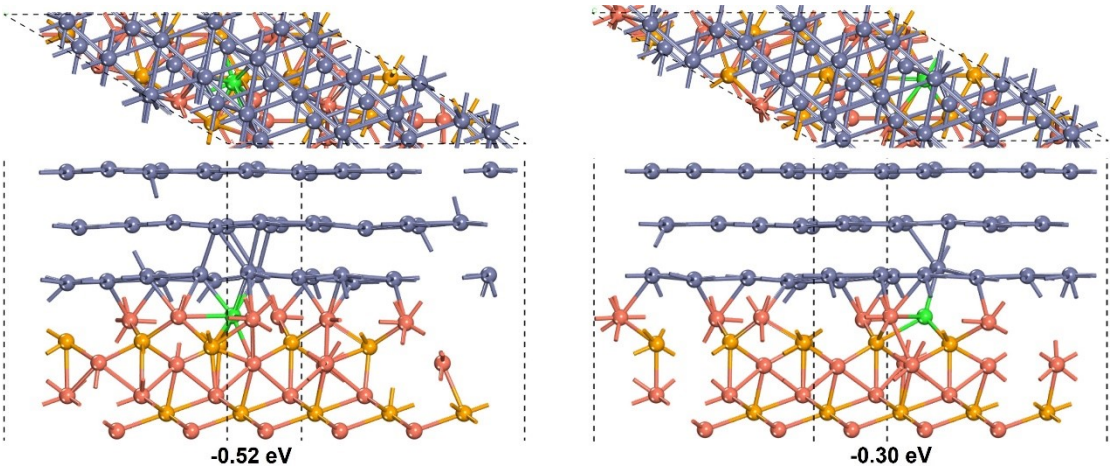

Figure S6. The top (up) and side (down) view of optimized adsorption configuration of Zn atom on the Zn(002)@Cu_2Se. Amber, coralito, green, and blue gray ball marks Se, Cu, Zn atom of the interface and bulk phase Zn, respectively.

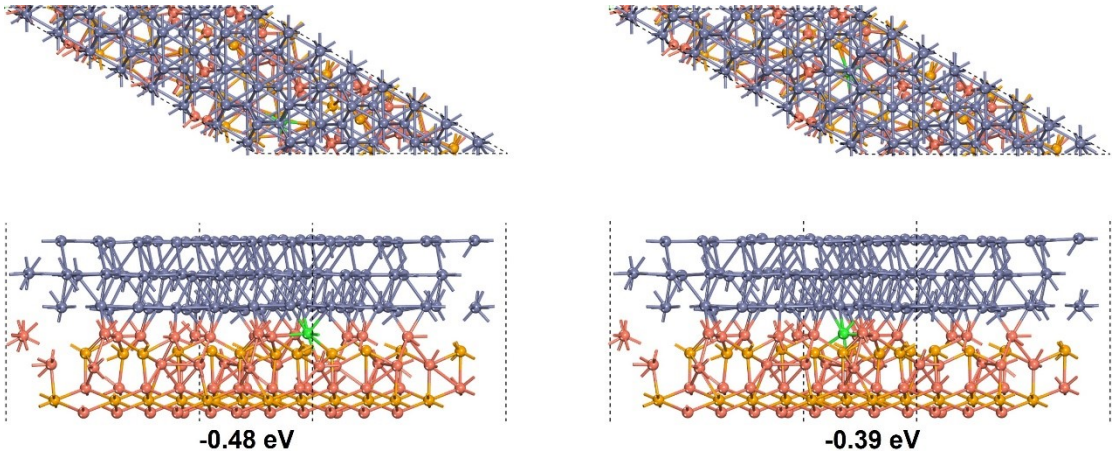

Figure S7. The top (up) and side (down) view of optimized adsorption configuration of Zn atom on the Zn(100)@Cu_2Se. Amber, coralito, green, and blue gray ball marks Se, Cu, Zn atom of the interface and bulk phase Zn, respectively.

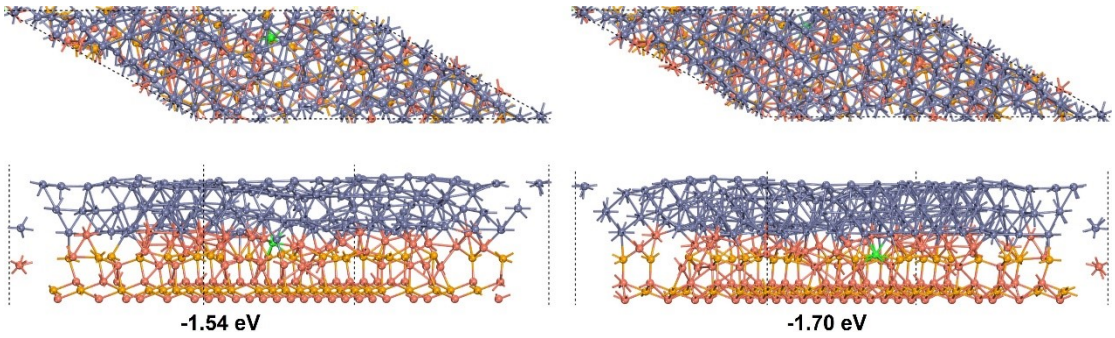

Figure S8. The top (up) and side (down) view of optimized adsorption configuration of Zn atom on the Zn(101)@Cu_2Se. Amber, coralito, green, and blue gray ball marks Se, Cu, Zn atom of the interface and bulk phase Zn, respectively.