Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for: Tuning the Structural Skeletal of a Phenanthroline-based Covalent Organic Framework for better Electrochemical Performance as Cathode Material for Zn-Ion Batteries: A Theoretical Exploration

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Supporting Information

1. The electronic band structure plot of PACOF.

2. The electronic band structure and charge density difference (CDD) plot of Zn(C_{NN})-adsorbed PACOF.

3. Another view of migration of zinc atoms on PACOF along the three diffusion pathways.

4. The electronic band structure plot of QPACOF

5. The electronic band structure and charge density difference (CDD) plot of Zn(C_{ON})-adsorbed QPACOF.

6. The route for the experimental synthesis of our predicted model system (QPACOF).

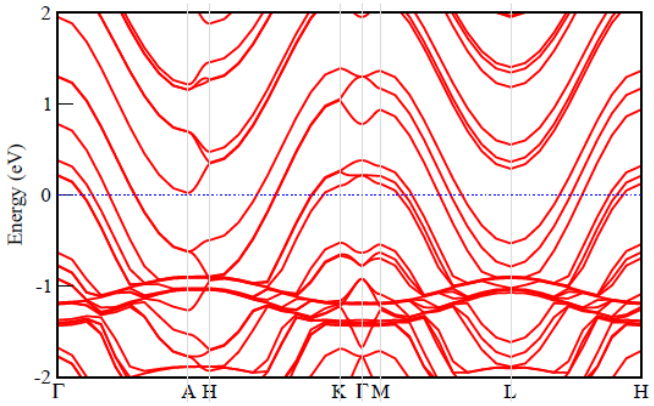

Figure S1: **Electronic band structure plot of PACOF. The Fermi level is indicated by the blue dashed line.**

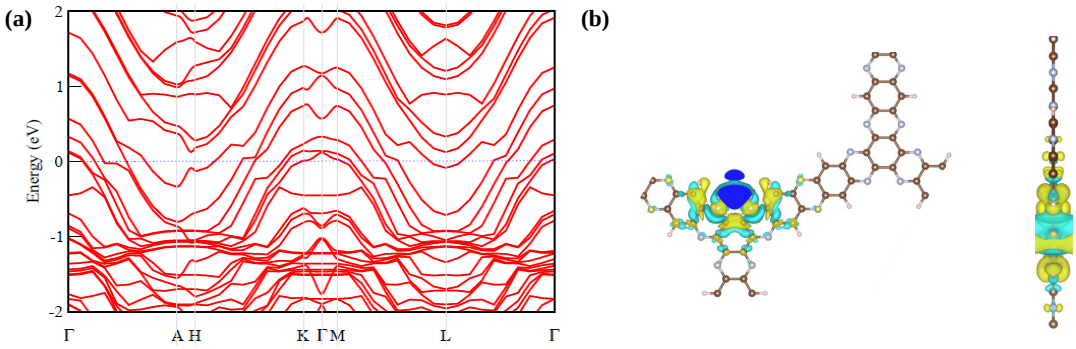

Figure S2: **(a) Electronic band structure plot of Zn(C_{NN})-adsorbed PACOF. The Fermi level is shown by blue dashed line. (b) Charge density difference (CDD) plot of Zn(C_{NN})-adsorbed PACOF.**

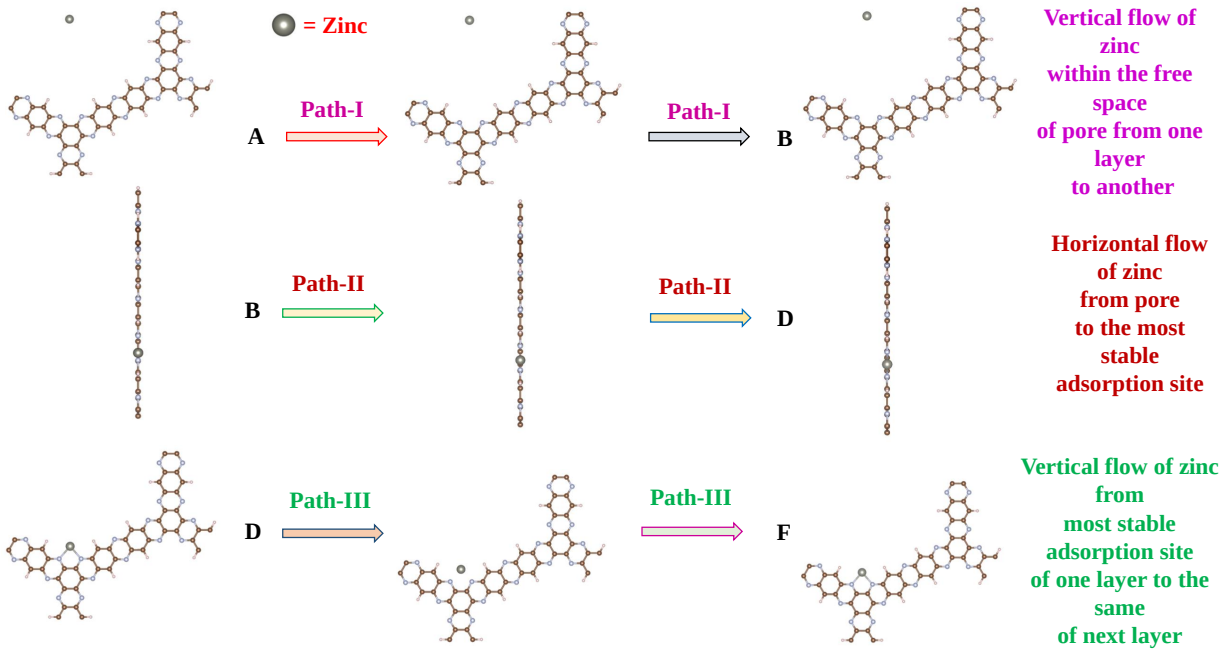

Figure S3: **Another view of migration of zinc atoms on PACOF along the three diffusion pathways.**

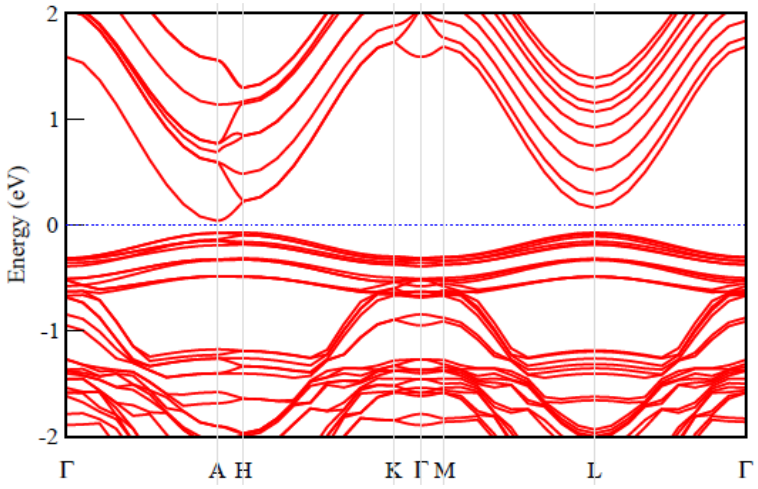

Figure S4: **Electronic band structure plot of QPACOF. The Fermi level is indicated by the blue dashed line.**

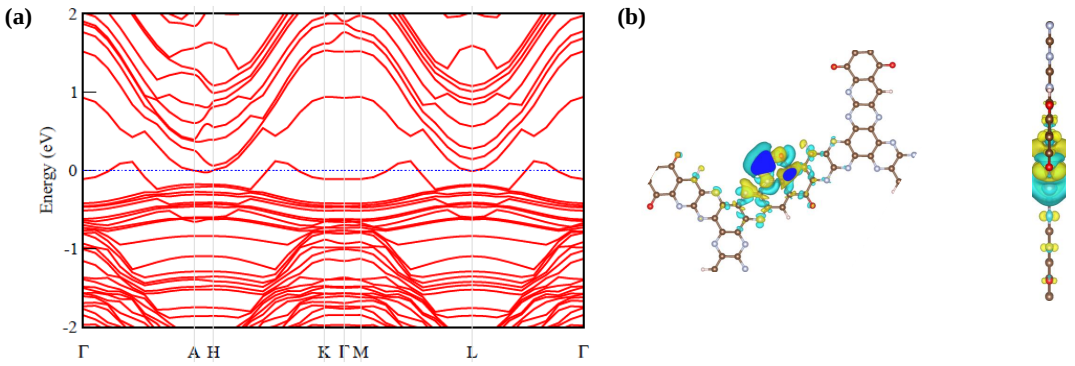

Figure S5: **(a) Electronic band structure plot of Zn(C_{ON})-adsorbed QPACOF. The Fermi level is shown by blue dashed line. (b) Charge density difference (CDD) plot of Zn(C_{ON})-adsorbed QPACOF.**

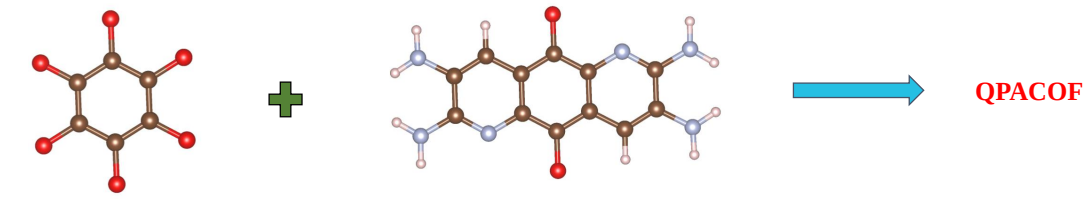

Figure S6: **Schematic diagram for the experimental synthesis of our proposed model system (QPACOF)**