

Supporting Information

Lithium-Ion Distribution and Motion in Two-Dimensional Covalent Organic Frameworks: The Example of TAPB-PDA COF

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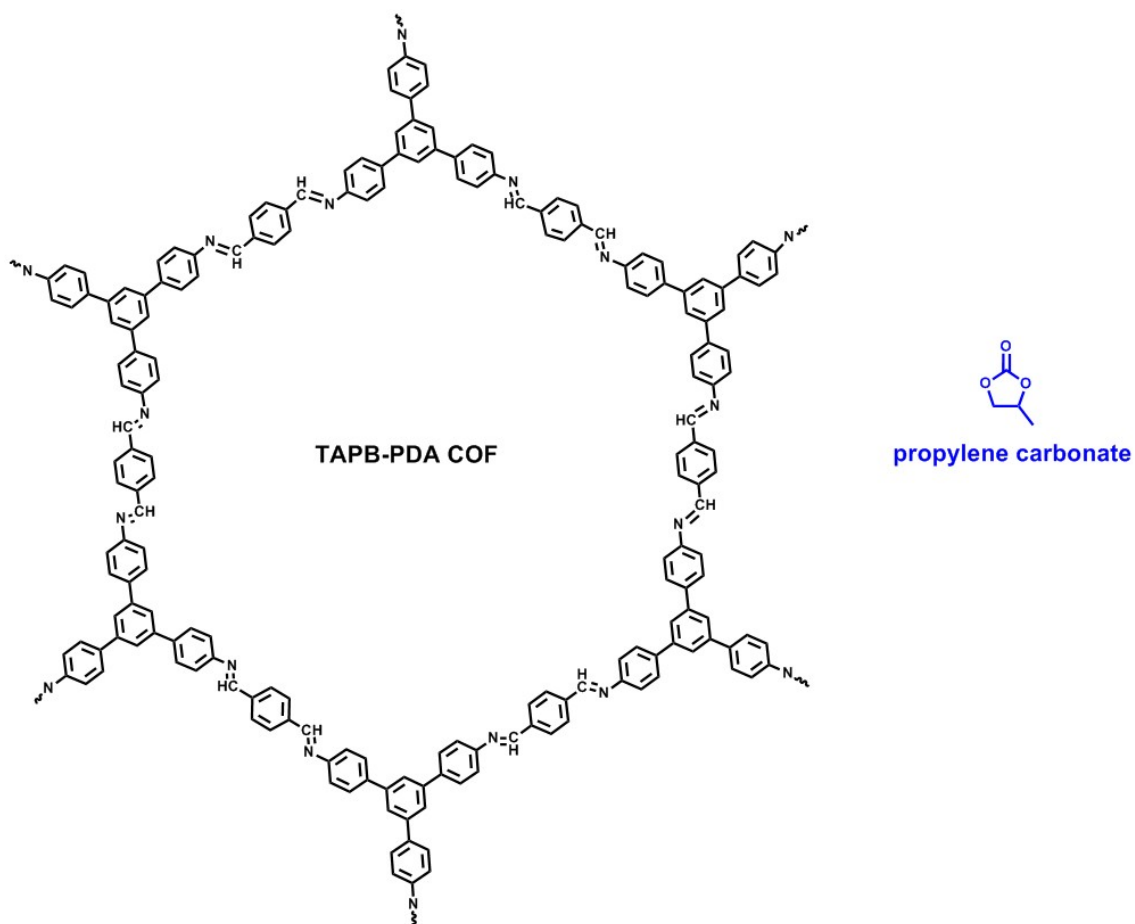


Figure S1. Chemical structures of TAPB-PDA COF and propylene carbonate.

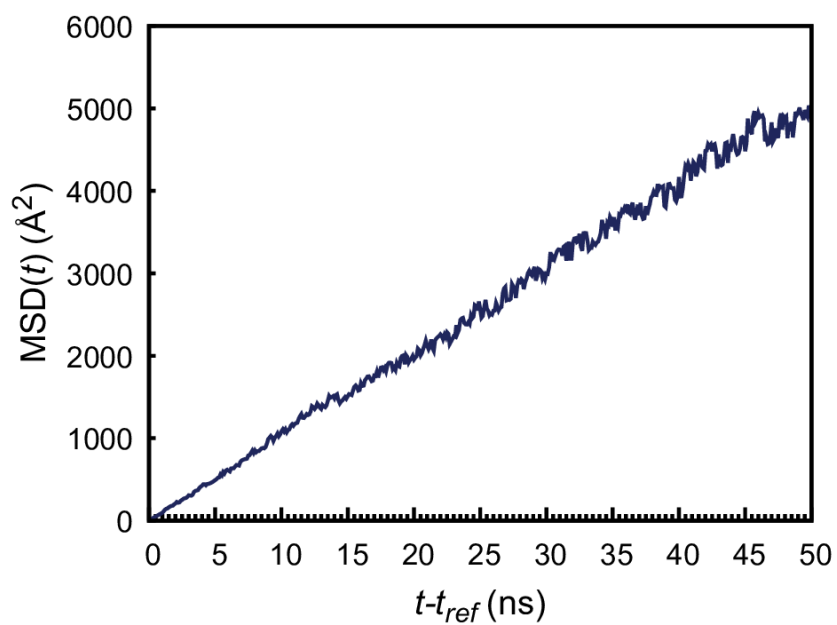


Figure S2. Mean square deviation of Li^+ in PC solution at 1 M LiClO_4 .

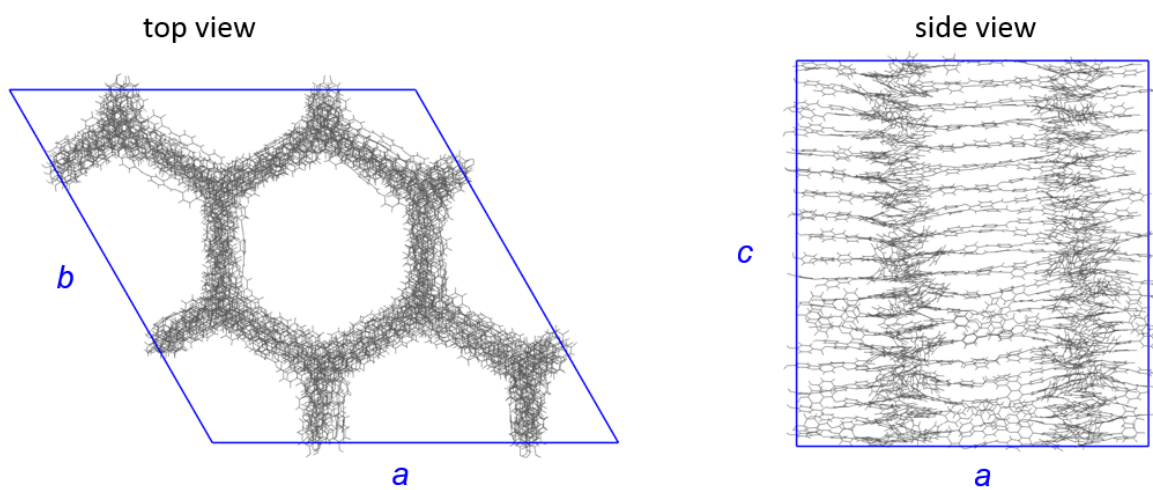


Figure S3. A representative snapshot of simulated TAPB-PDA COF without LiClO_4 .

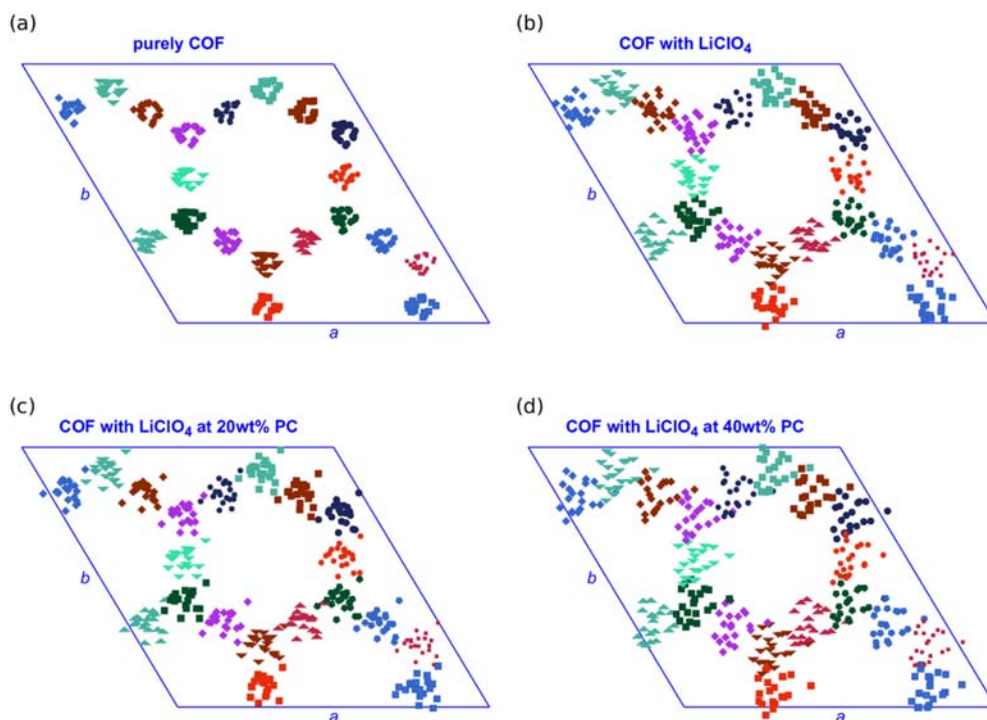


Figure S4. Projection of the coordinates of monomer units of the simulated COF onto the *ab*-plane for different systems: (a) purely TAPB-PDA COF without LiClO₄ and TAPB-PDA COF mixed with LiClO₄ at (b) 0wt%, (c) 20wt% and (d) 40wt% PC. Dots of the same color and shape represent the monomer units initially stacked at the same location in the *ab*-plane.

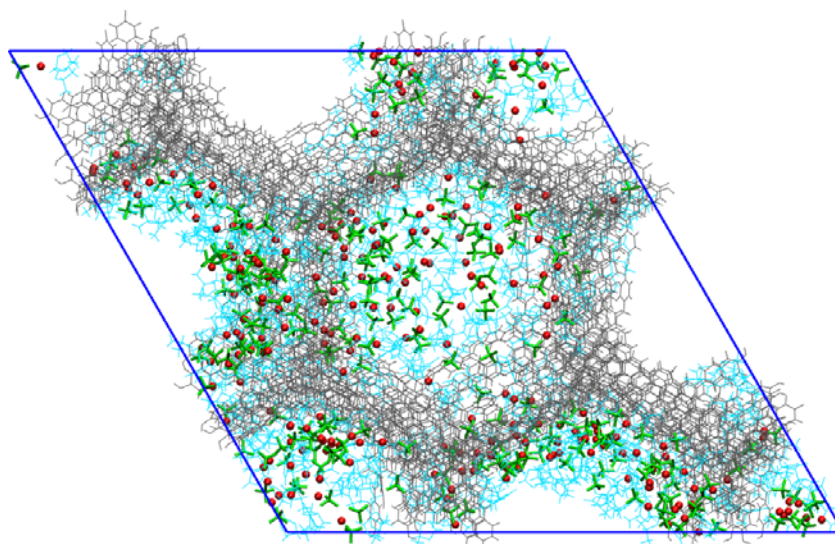


Figure S5. Top view at 200 ns for TAPB-PDA COF mixed with LiClO₄ at 30wt% PC. Red spheres, green rods and cyan lines represent Li⁺, ClO₄⁻ and PC molecules, respectively.

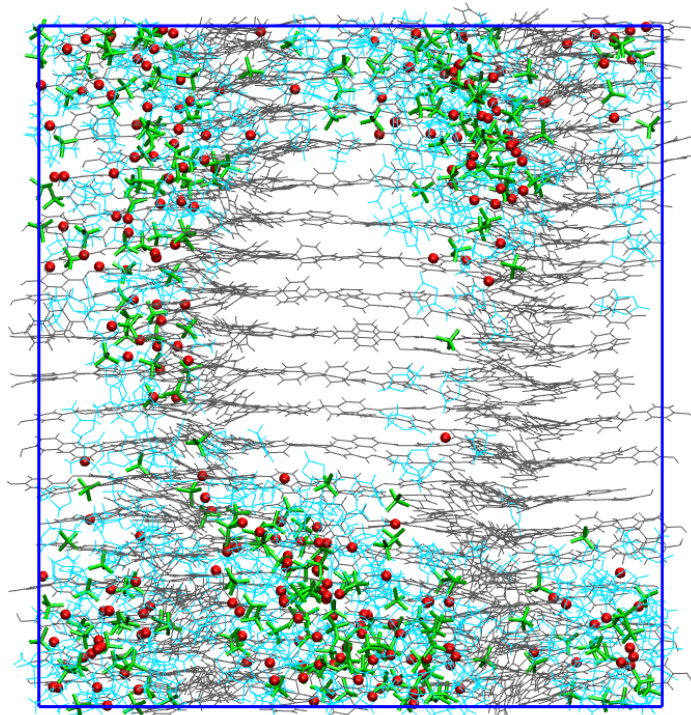


Figure S6. Side view at 200 ns for TAPB-PDA COF mixed with LiClO₄ at 30wt% PC. Red spheres, green rods and cyan lines represent Li⁺, ClO₄⁻ and PC molecules, respectively.

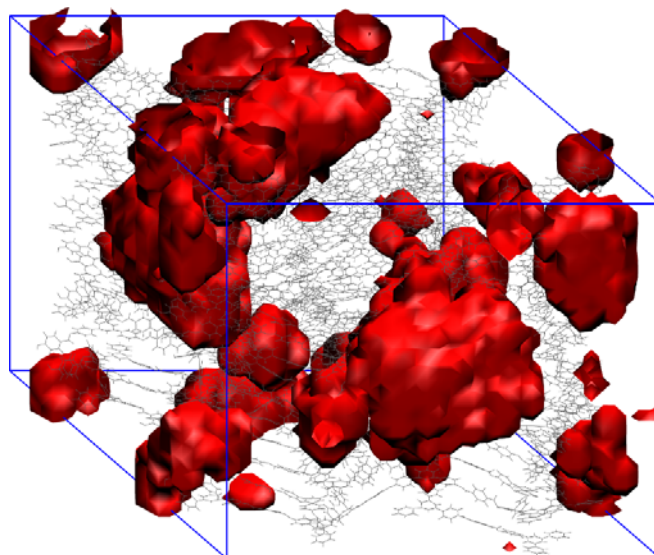


Figure S7. Illustrations of the occupations of Li⁺ at 10wt% PC. The isosurfaces denote the boundaries of a 99% probability of presence in the last 100 ns-trajectory.

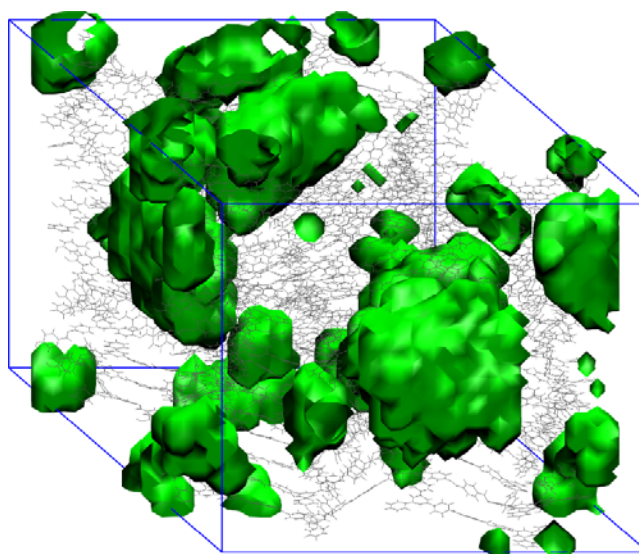


Figure S8. Illustrations of the occupations of ClO_4^- at 10wt% PC. The isosurfaces denote the boundaries of a 99% probability of presence in the last 100 ns-trajectory.

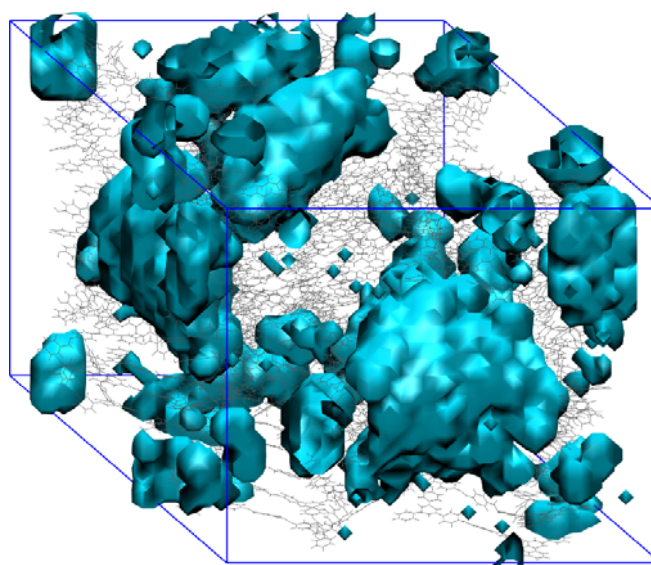


Figure S9. Illustrations of the occupations of PC at 10wt% PC. The isosurfaces denote the boundaries of a 99% probability of presence in the last 100 ns-trajectory.

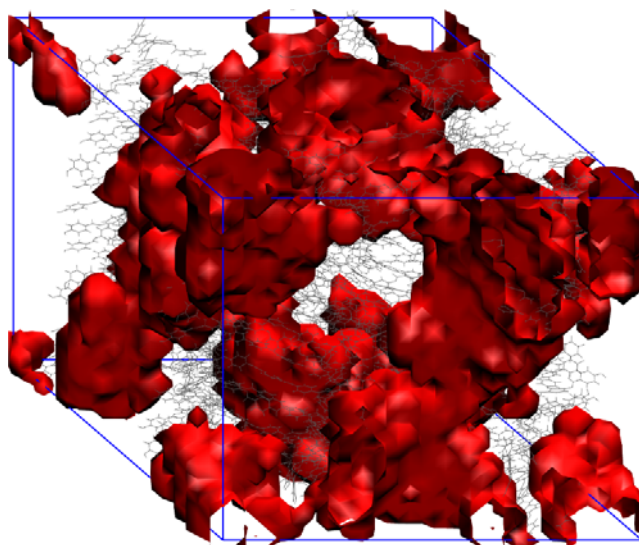


Figure S10. Illustrations of the occupations of Li^+ at 30wt% PC. The isosurfaces denote the boundaries of a 99% probability of presence in the last 100 ns-trajectory.

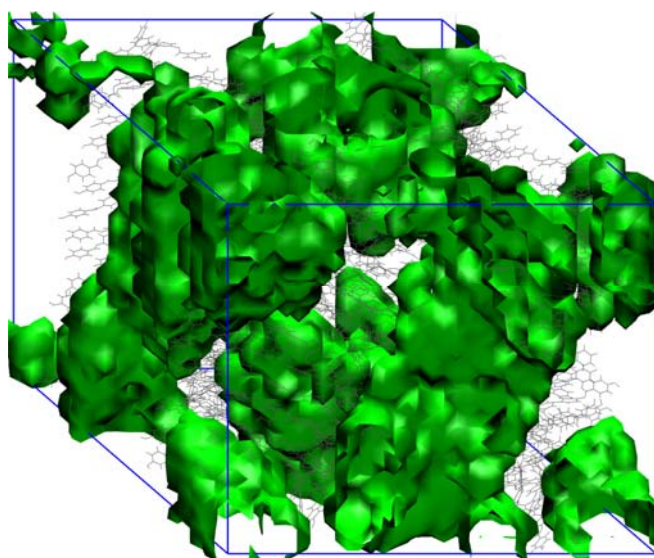


Figure S11. Illustrations of the occupations of ClO_4^- at 30wt% PC. The isosurfaces denote the boundaries of a 99% probability of presence in the last 100 ns-trajectory.

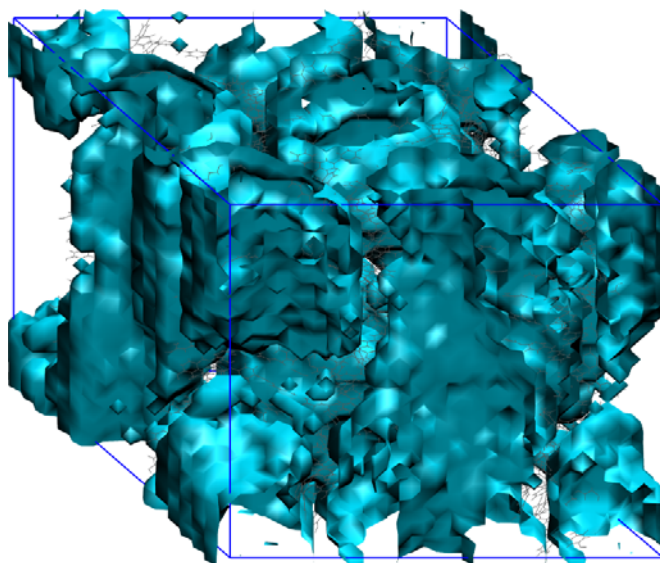


Figure S12. Illustrations of the occupations of PC at 30wt% PC. The isosurfaces denote the boundaries of a 99% probability of presence in the last 100 ns-trajectory.