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 LiClO$_4$ and TAPB-PDA COF mixed with LiClO$_4$ 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 LiClO$_4$ at 30wt% PC. Red spheres, green rods and cyan lines represent Li$^+$, ClO$_4^-$ and PC molecules, respectively.
Figure S6. Side view at 200 ns for TAPB-PDA COF mixed with LiClO$_4$ at 30wt% PC. Red spheres, green rods and cyan lines represent Li$^+$, ClO$_4^-$ 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 ClO₄⁻ 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.