

# Diffusion mechanisms in smectic ionic liquid crystals: insights from coarse-grained MD simulations

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## Electronic Supporting Information

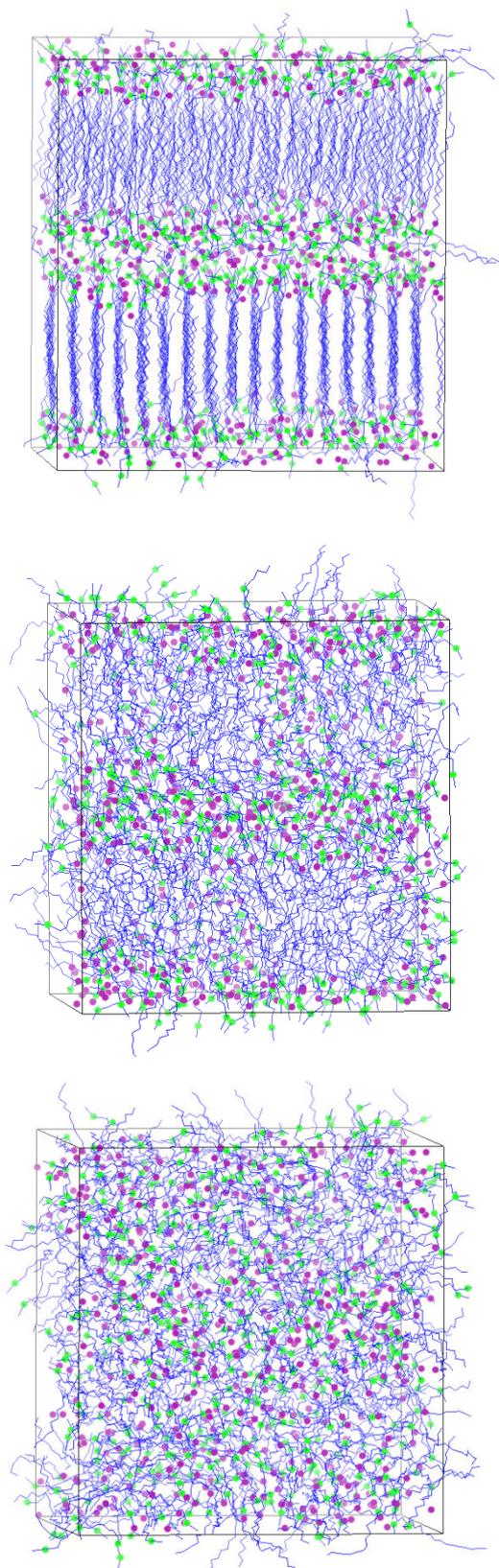


Figure 1: Snapshots of the simulation box representing the three phases. From top to bottom: CrB at 450 K, SmA at 505 K and Iso at 600 K. Cation heads (site A) in green, anions (site D) in purple and alkyl carbons (sites B, M1-M4, C, E) in blue.

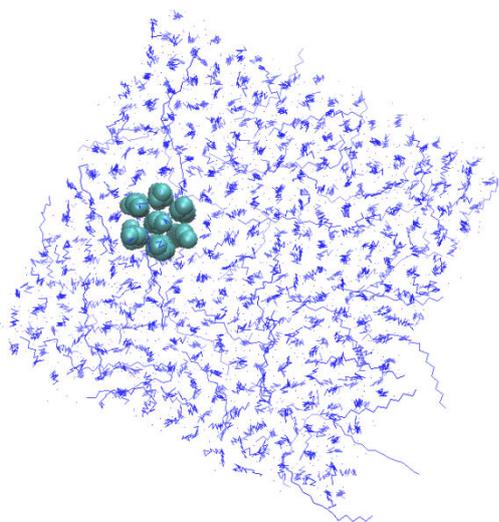


Figure 2: Snapshot of the simulation box at 450 K highlighting the hexagonal packing of alkyl chains.

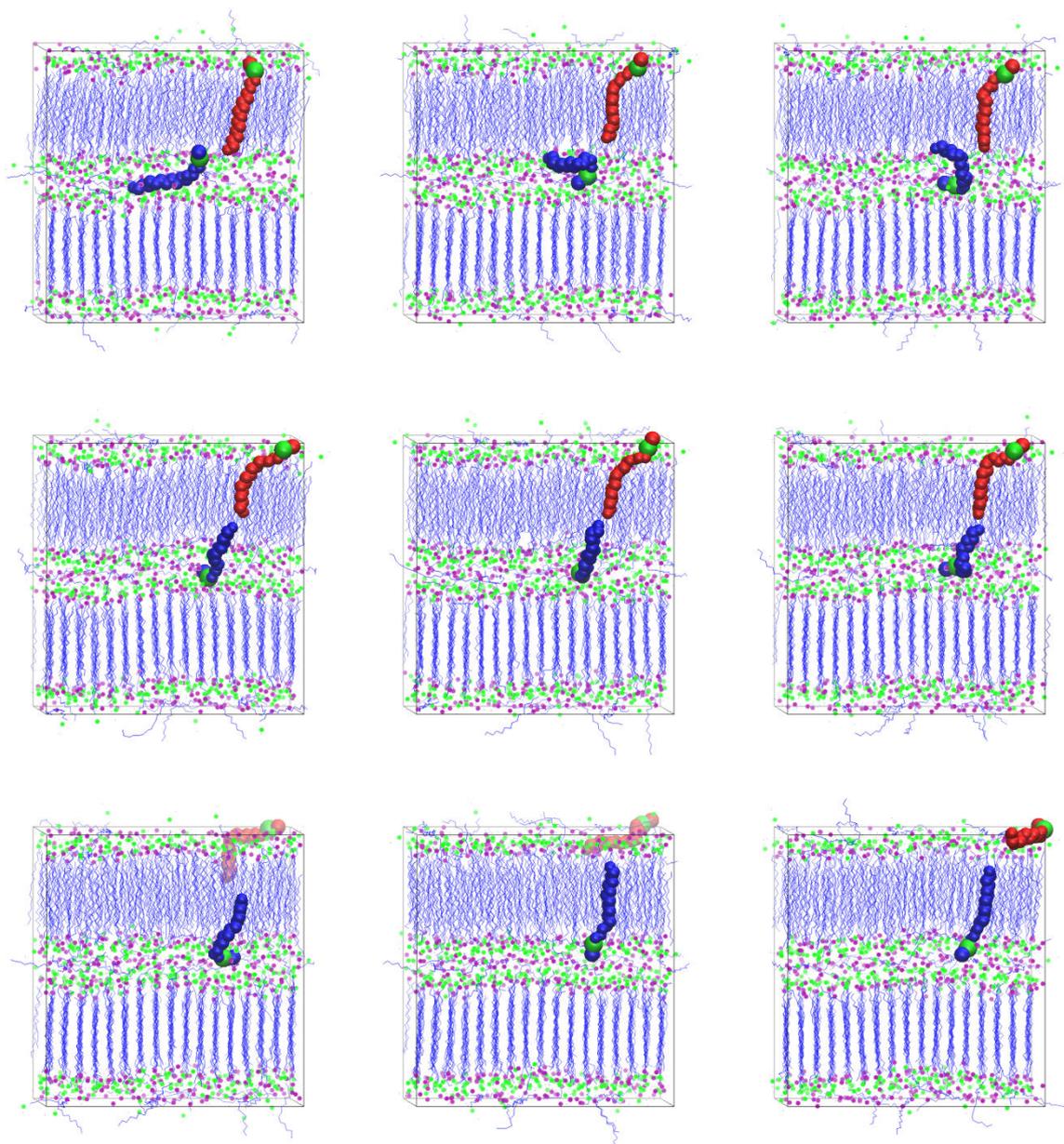


Figure 3: snapshots of the trajectories of Figure 4 of the main text taken at times (from top-left, to bottom-right): 5.4 ns; 11.07 ns; 11.15 ns; 11.21 ns; 11.26 ns; 11.34 ns; 11.48 ns; 11.50 ns; 15.82 ns.

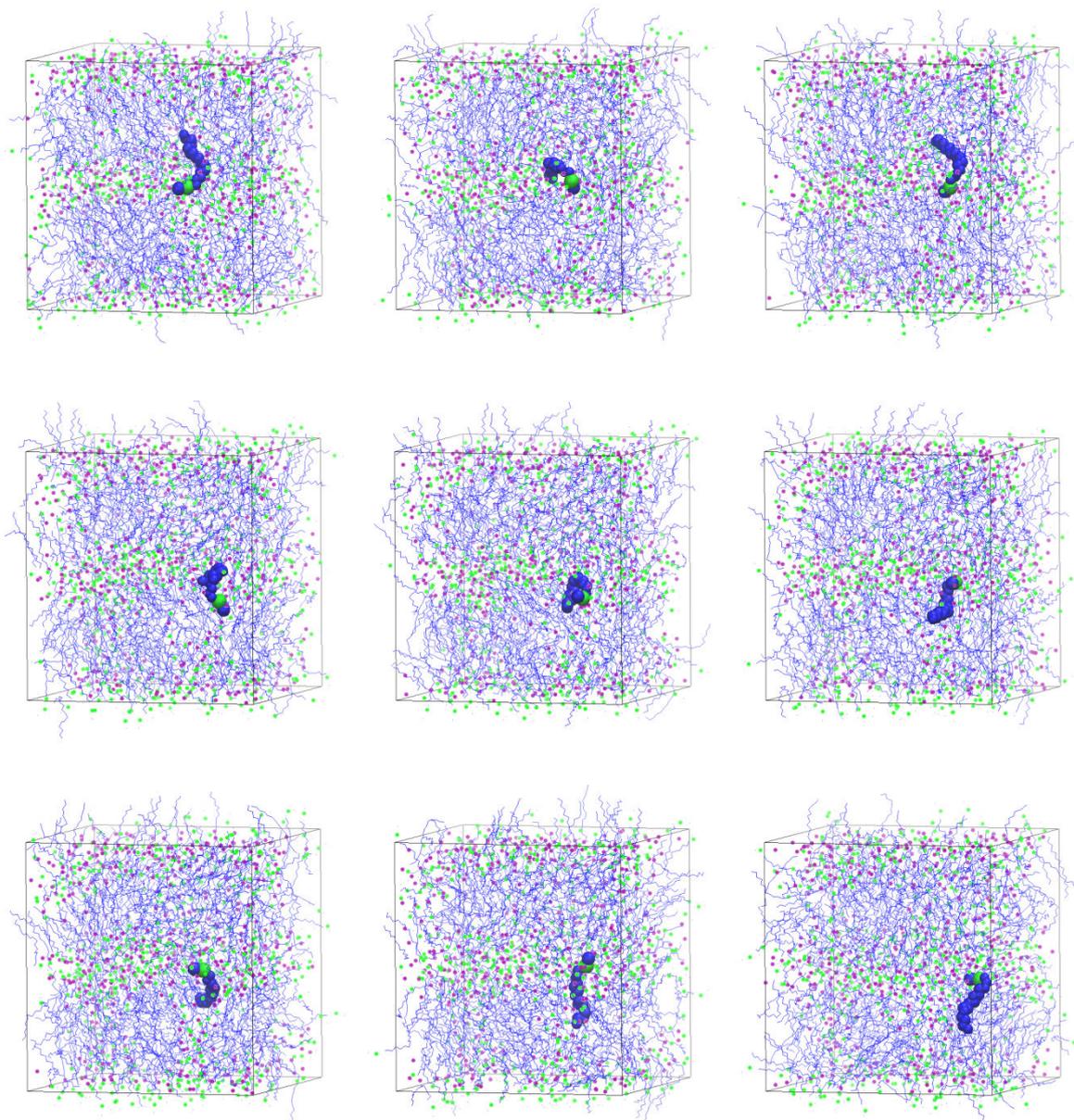


Figure 4: Snapshots of one of the trajectories of Figure 6 of the main text (blue line) taken at times (from top-left, to bottom-right): 6.75 ns; 8.37 ns; 8.56 ns; 8.69 ns; 8.72 ns; 8.75 ns; 8.80 ns; 8.86 ns; 10.80 ns. The mechanism highlighted is similar to that one operating in the crystal B phase with the cation head remaining into the same layer.

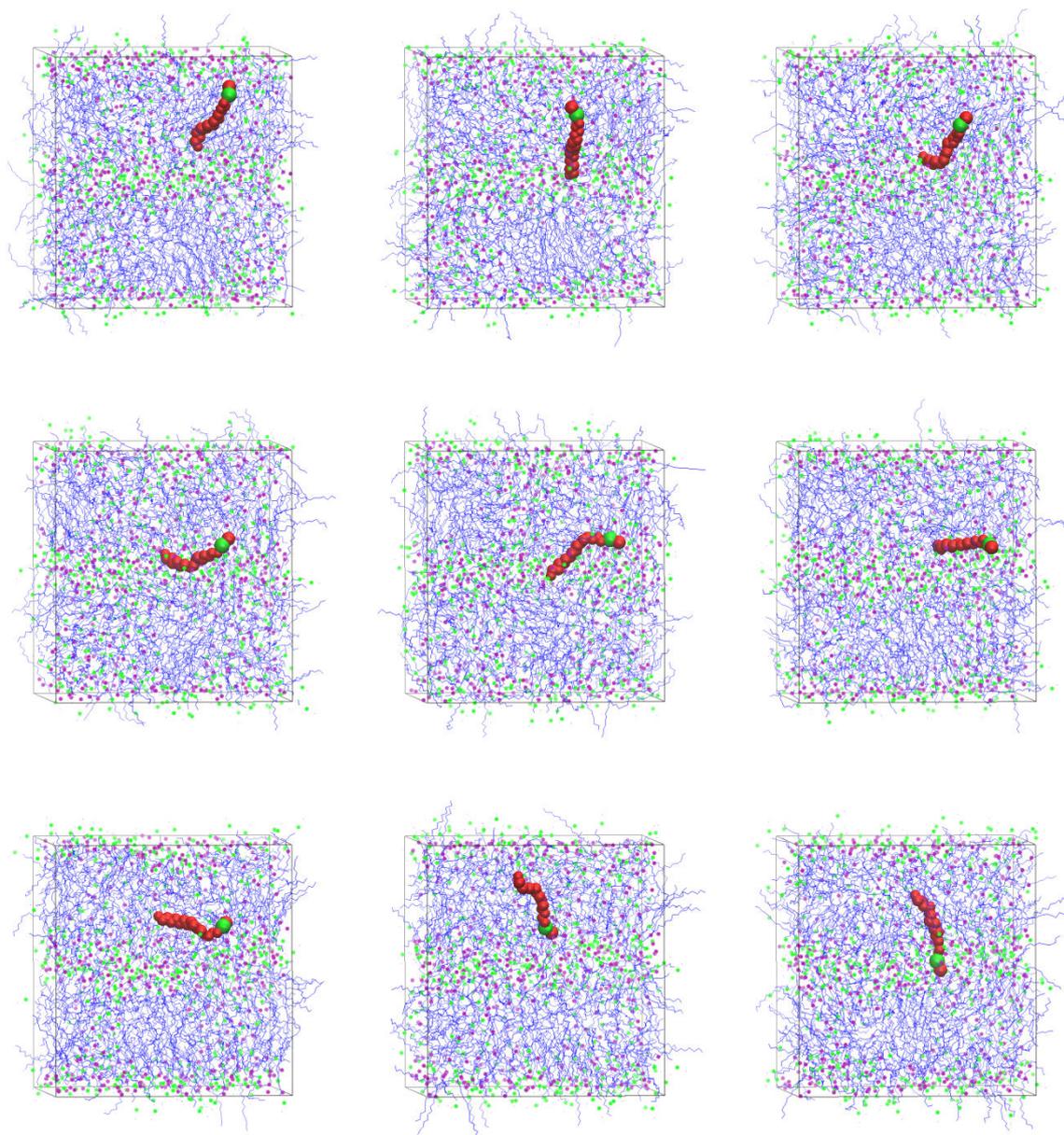


Figure 5: Snapshots of one of the trajectories of Figure 6 of the main text (red line) taken at times (from top-left, to bottom-right): 13.50 ns; 13.77 ns; 14.04 ns; 14.31 ns; 14.58 ns; 14.85 ns; 15.12 ns; 15.39 ns; 15.66 ns. The mechanism highlighted is a direct permeation through the hydrophobic layer followed by a reorientation.