Electronic Supplementary Material (ESI) for Nanoscale

Supporting Information

"Rupture mechanism of liquid crystal thin films realized by large-scale molecular simulations"

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Visualization method

- We implemented a path tracer that supports lighting, materials, depth cueing, motion blur and shadows for multi-million particle systems.
- Simulation snapshots are generated from offline simulation data.
- MD trajectories are visualized using the OLCF Visualization Laboratory facility.

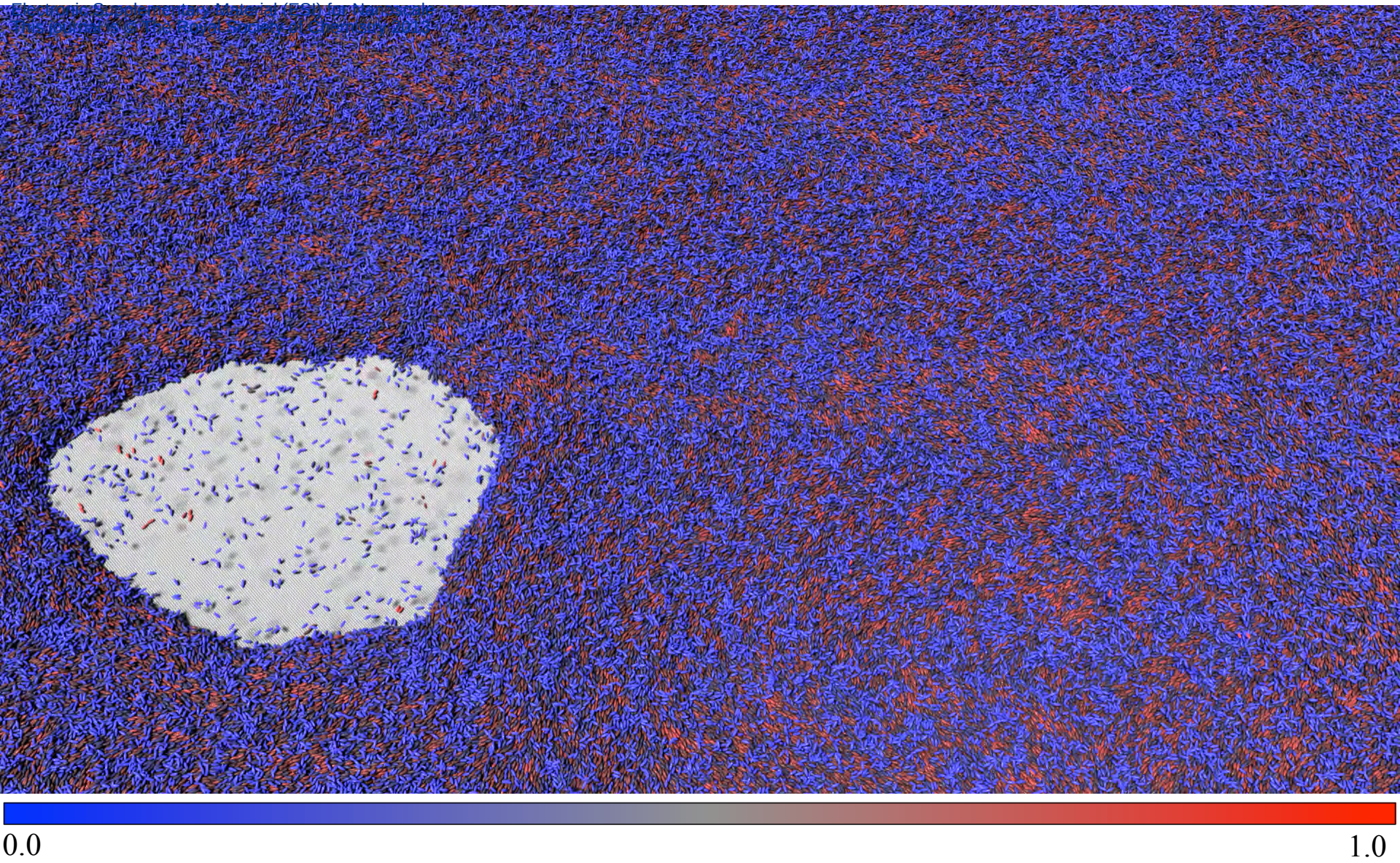

Figure S1: Zoomed-in perspective view of a hole in the nematic $h_0 = 8.0\sigma_0$ film: LC mesogens are colored by their local alignment parameter: red = good local alignment with their neighbors, blue = poor alignment. Substrate particles are not shown. Only LC mesogens in the liquid phase ($z < 12.0\sigma_0$) are visualized.

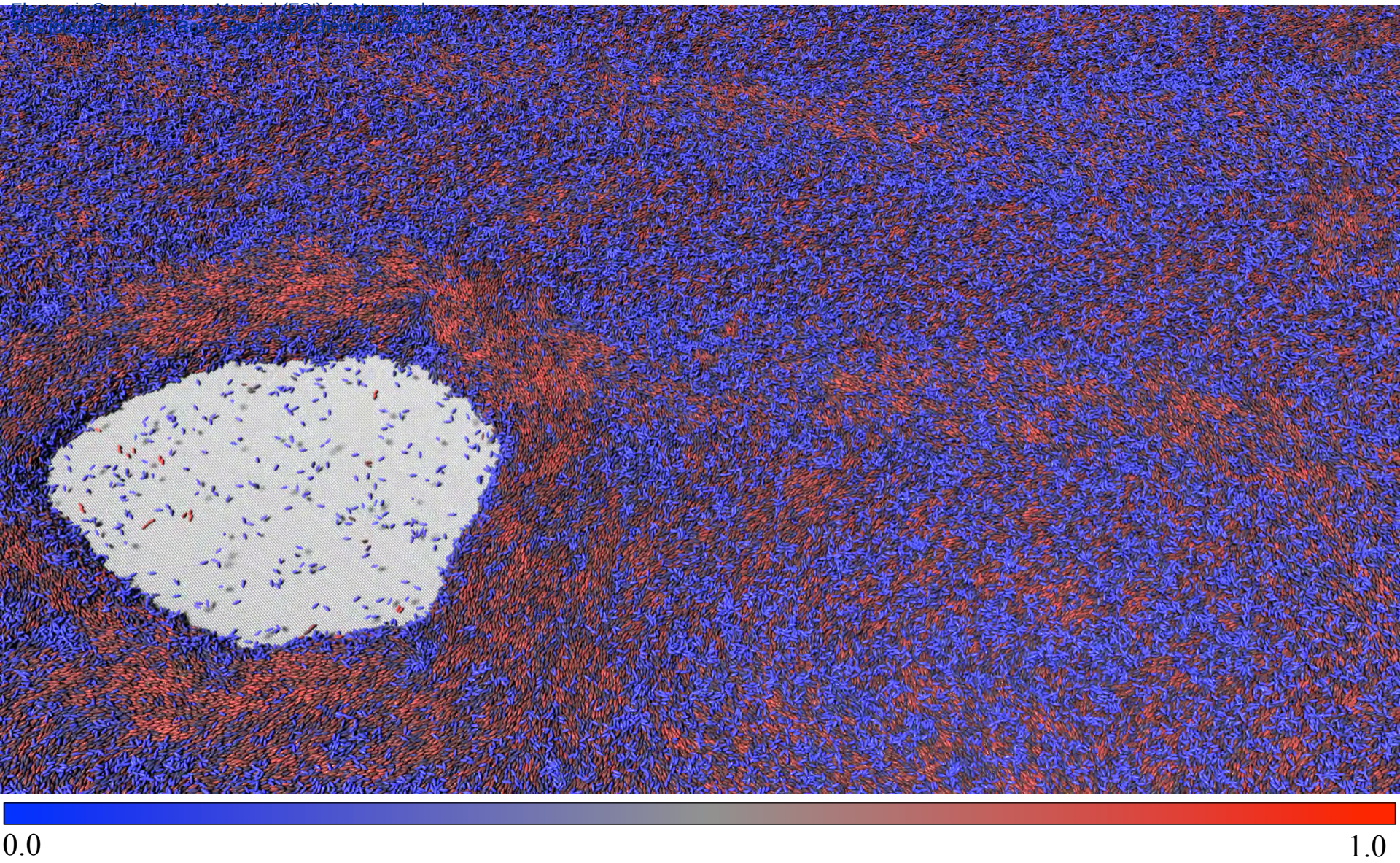

Figure S2: Zoomed-in perspective view of a hole in the nematic $h_0 = 8.0\sigma_0$ film: LC mesogens are colored by their local alignment parameter: red = good local alignment with their neighbors, blue = poor alignment. Substrate particles are not shown. Only LC mesogens with $z < 9.0\sigma_0$ are visualized to further reveal the orientational odering within the liquid phase.

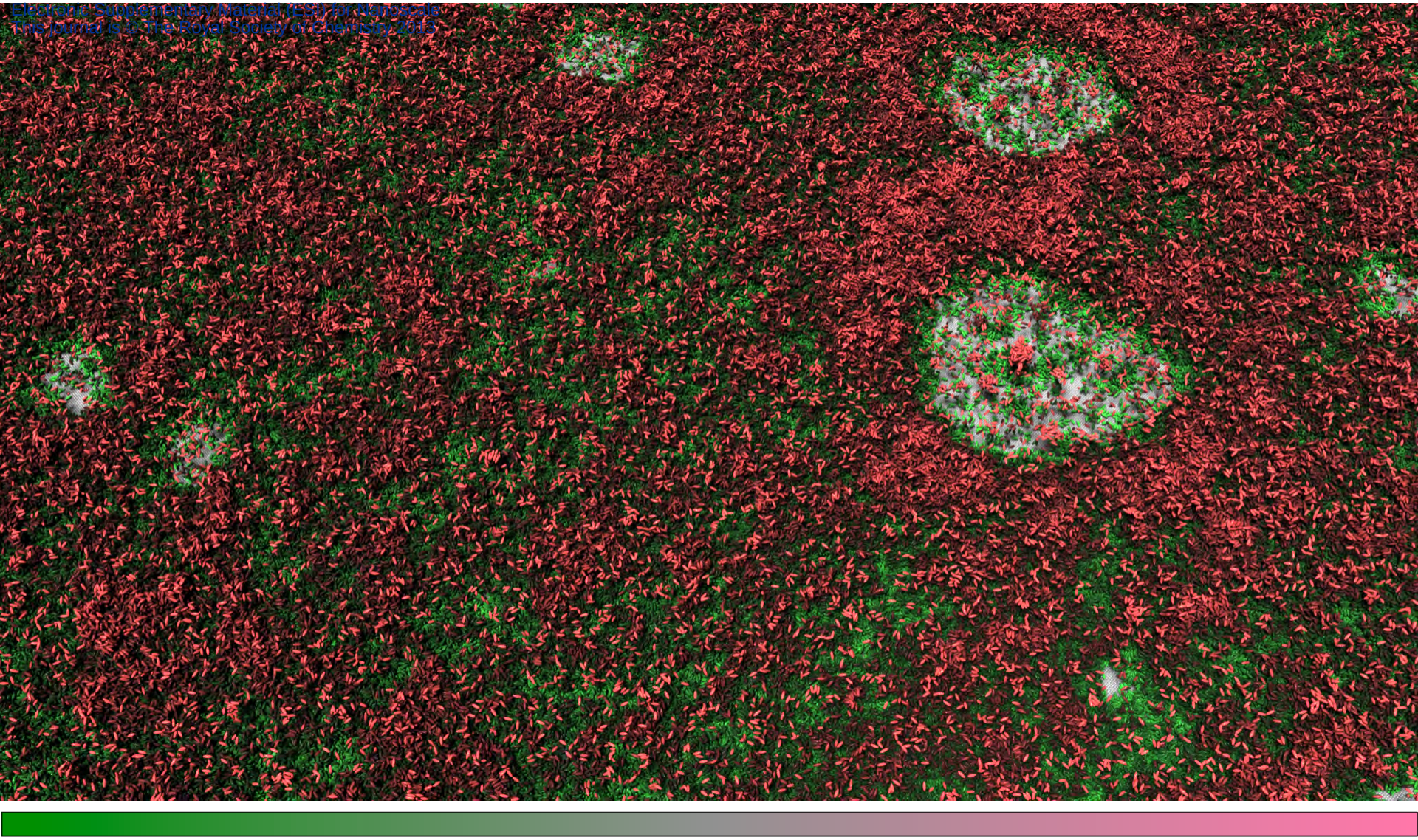

Figure S3: Zoomed-in perspective view of the isotropic $h_0 = 8.0\sigma_0$ film: LC mesogens are colored by their z coordinate. Substrate particles are not shown. Only LC mesogens with $z < 12.0\sigma_0$ are visualized.