Electronic Supplementary Material (ESI) for Soft Matter

MD simulation of the mesomorphic behaviour of 1-hexadecyl-3-methylimidazolium nitrate: assessment of the performance of a Coarse-Grained Force Field.

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Electronic Supporting Information

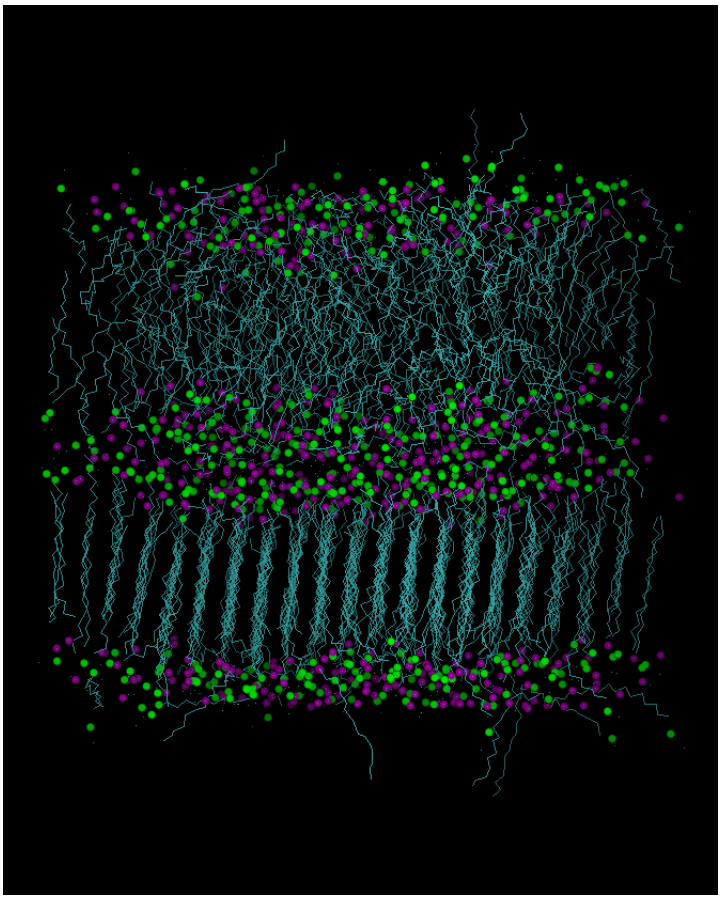

Figure 1. Snapshot of the box obtained at the end of the NPT simulation at 500 K showing the co-existence of a crystalline layer (bottom) and a smectic-like layer (top).

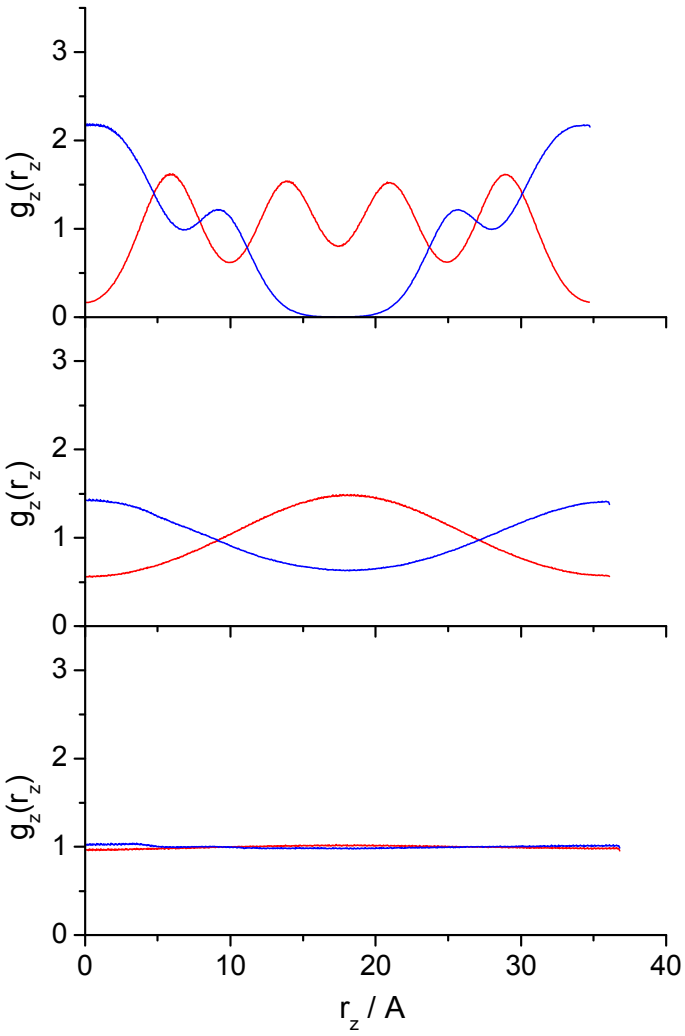

Figure 2.Cross pair distribution functions of the distance projected onto the *z* axis (the director orientation) at (from top to bottom) 450 K, 505 K and 600 K. Red AE sites; blue: AD sites.

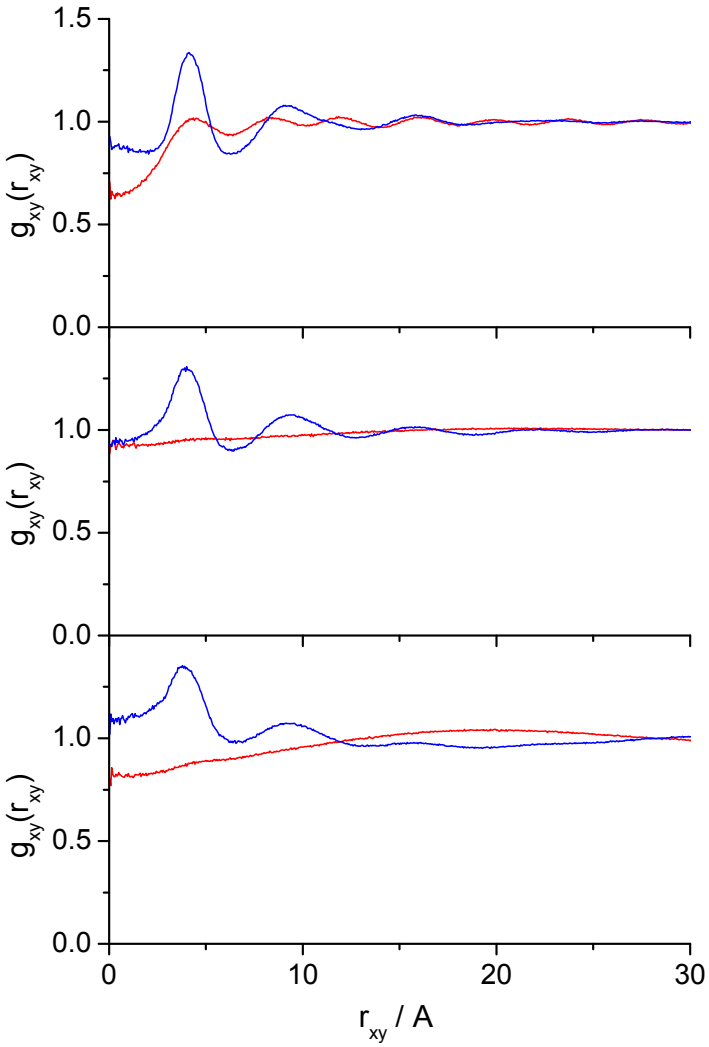

Figure 3. Cross pair distribution functions of the distance projected onto the *xy* plane (the normal to the director) at (from top to bottom) 450 K, 505 K and 600 K. Red AE sites; blue: AD sites.

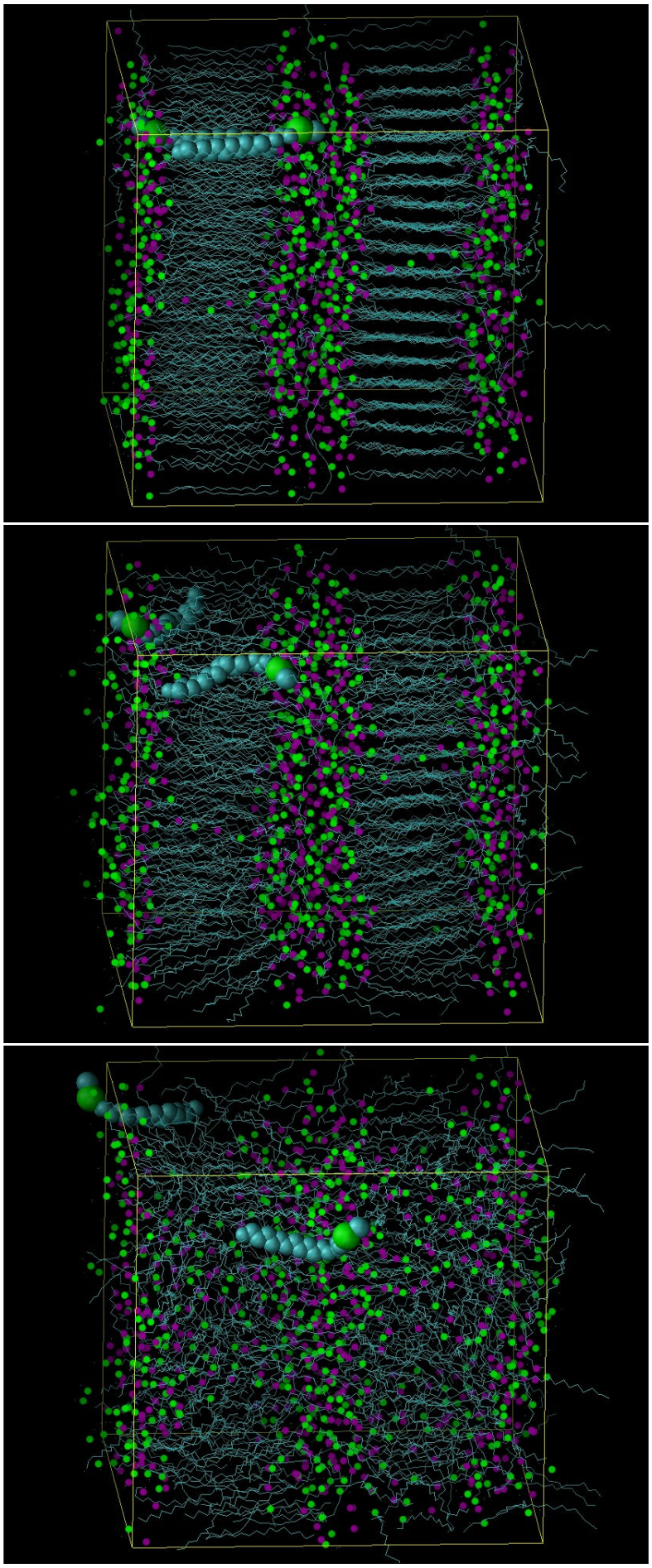

Figure 4. Snapshots taken after lowering the temperature at 470 K starting from the final configuration of the run equilibrated at 505 K. From left to right snapshots taken at 0 ns, 12 ns and 25 ns, respectively.

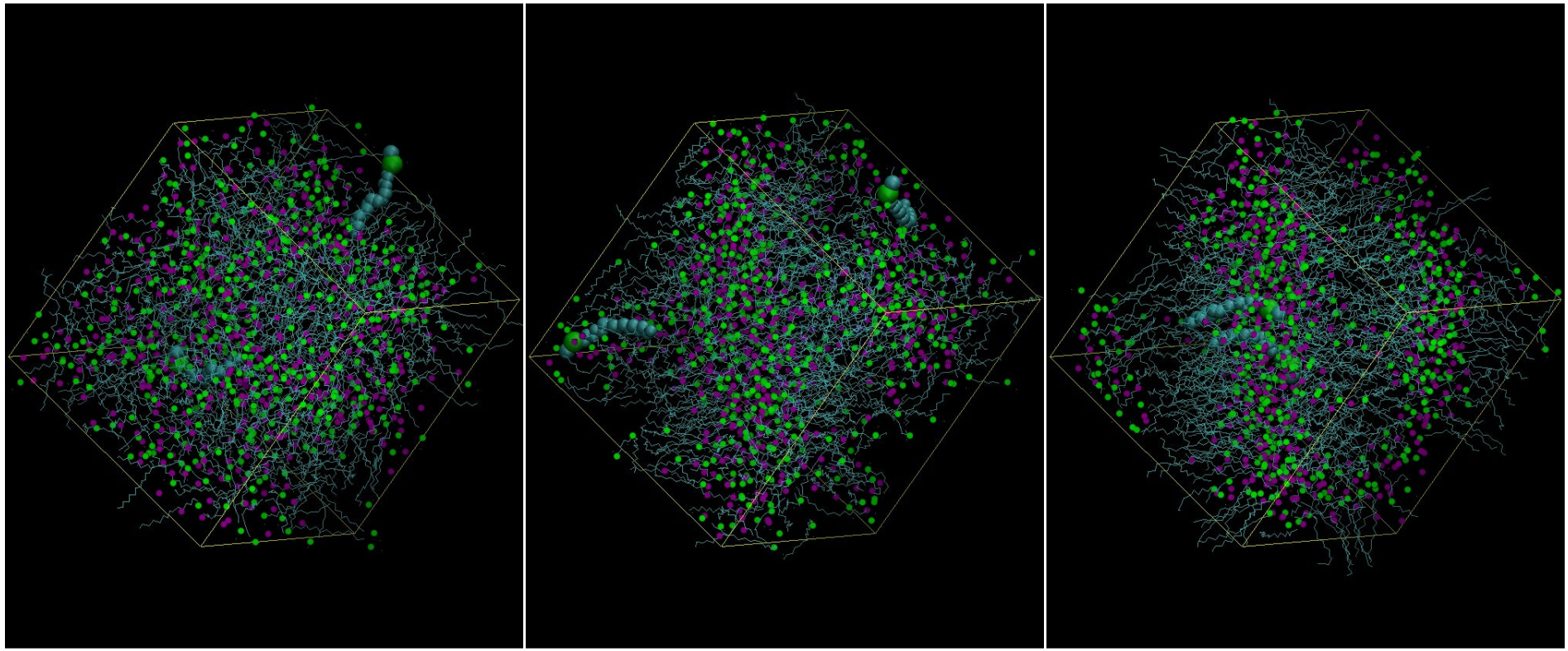

Figure 5. snapshots taken after lowering the temperature at 505 K starting from the final configuration of the run equilibrated at 600 K. From left to right snapshots taken at 0 ns, 25 ns and 50 ns, respectively. The system has been further equilibrated for more than 100 ns, remaining in the SmA phase.