Electronic Supplementary Material (ESI) for Soft Matter.

Supporting Information

A framework for multi-scale simulation of crystal growth in the presence of polymers

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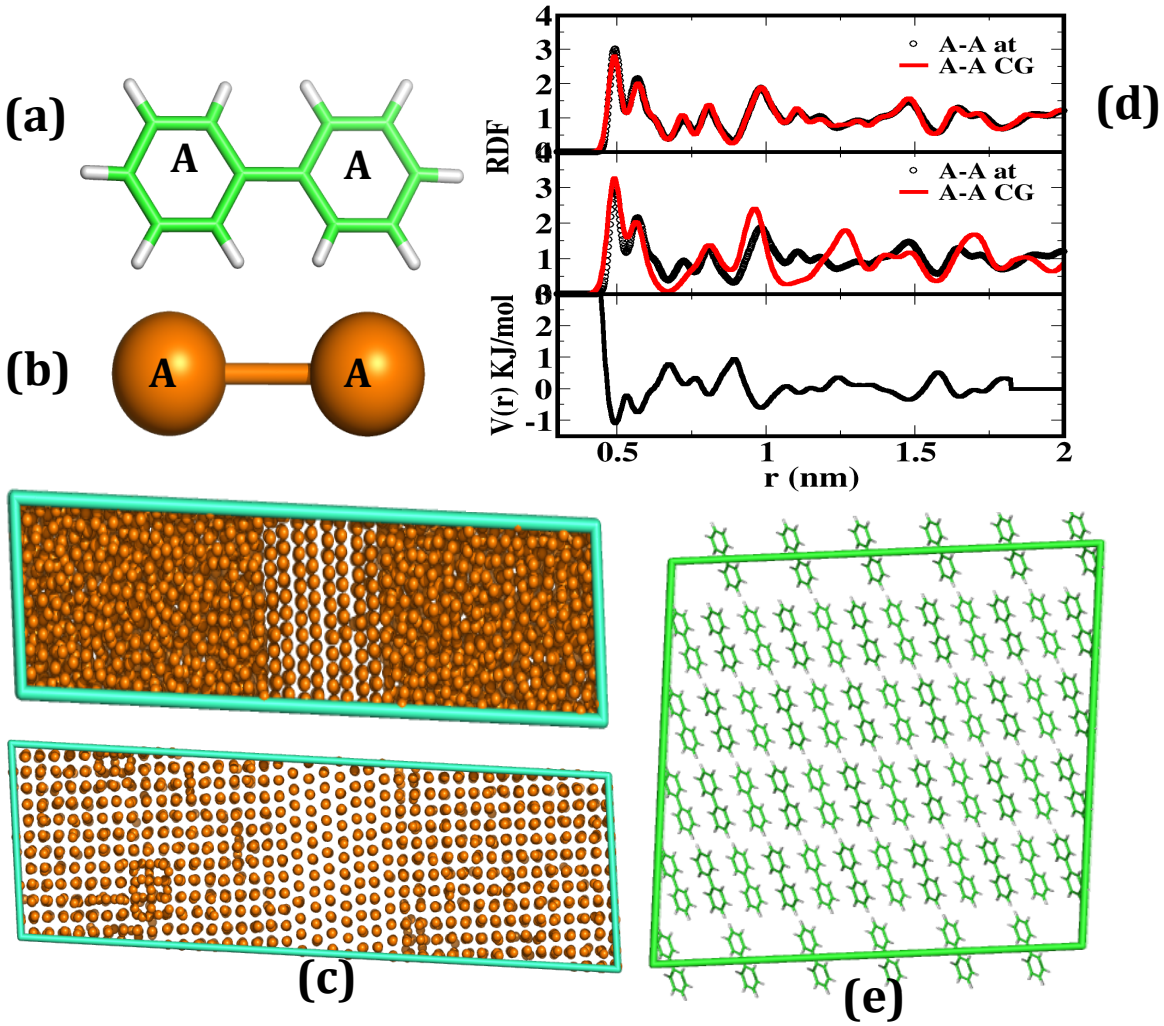

Figure S1: (a) atomistic representation of the biphenyl molecule (b) CG representation of the biphenyl molecule (c) *upper panel*: initial configuration of the crystalline slab in between two molten layers *lower panel*: final configuration of the grown structure. (d)

Comparison of the CG RDF with atomistic RDF for a preformed bulk structure (*upper panel*) and for the structure grown from melt (*middle panel*). *Lower panel*: potential of the CG bead. 'at' and 'CG' on the figure level stand for atomistic and coarse-grained, respectively. (e) Crystal structure of biphenyl.

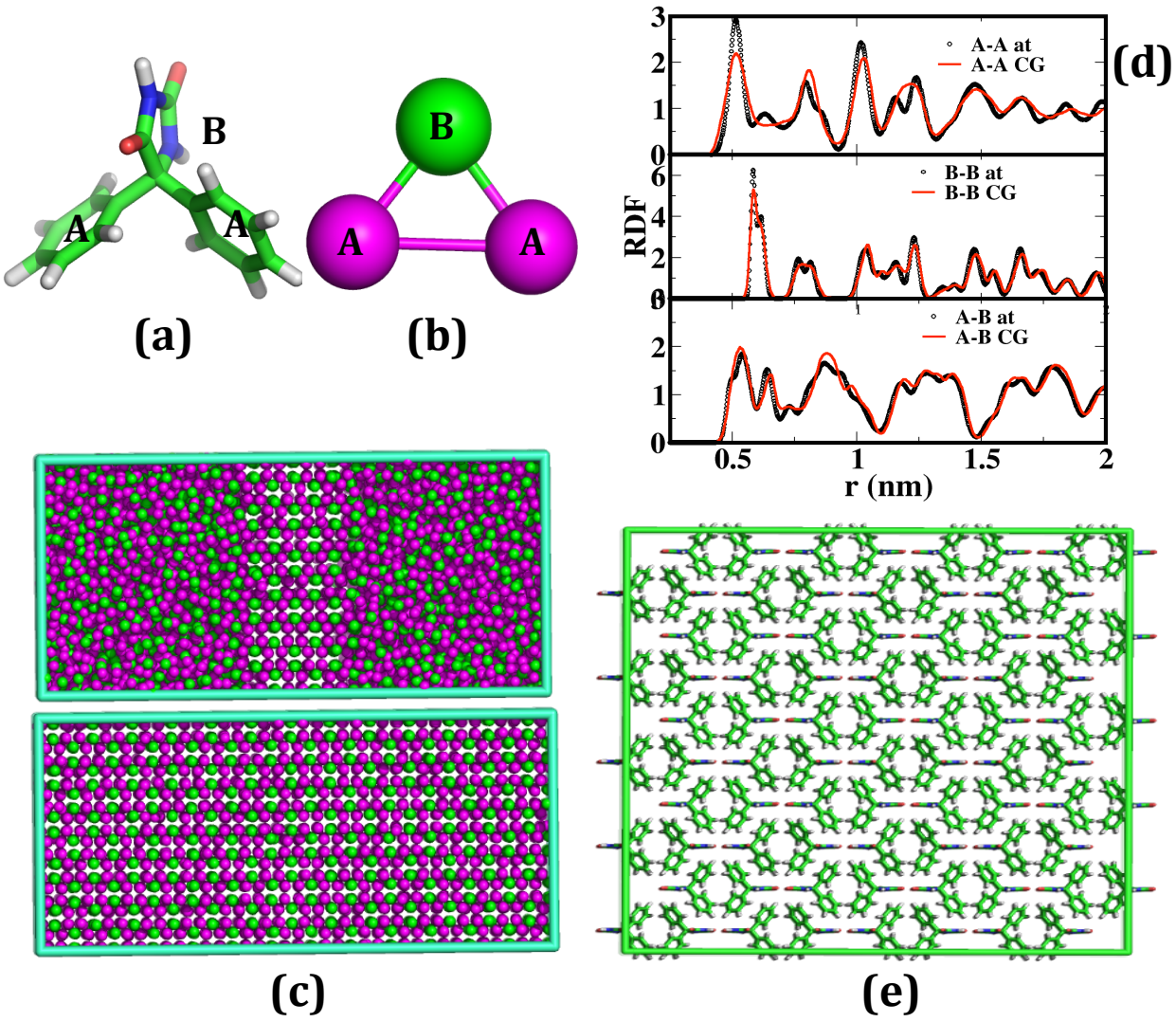

Figure S2: (a) atomistic representation of the phenytoin molecule (b) CG representation of the phenytoin molecule (c) *upper panel*: initial configuration of the crystalline slab in between two molten layers *lower panel*: final configuration of the grown structure. (d) Comparison of the RDFs of the CG beads with atomistic RDFs for the crystal structure

grown from the melt. ‘at’ and ‘CG’ on the figure level stand for atomistic and coarse-grained, respectively. (e) Crystal structure of phenytoin.

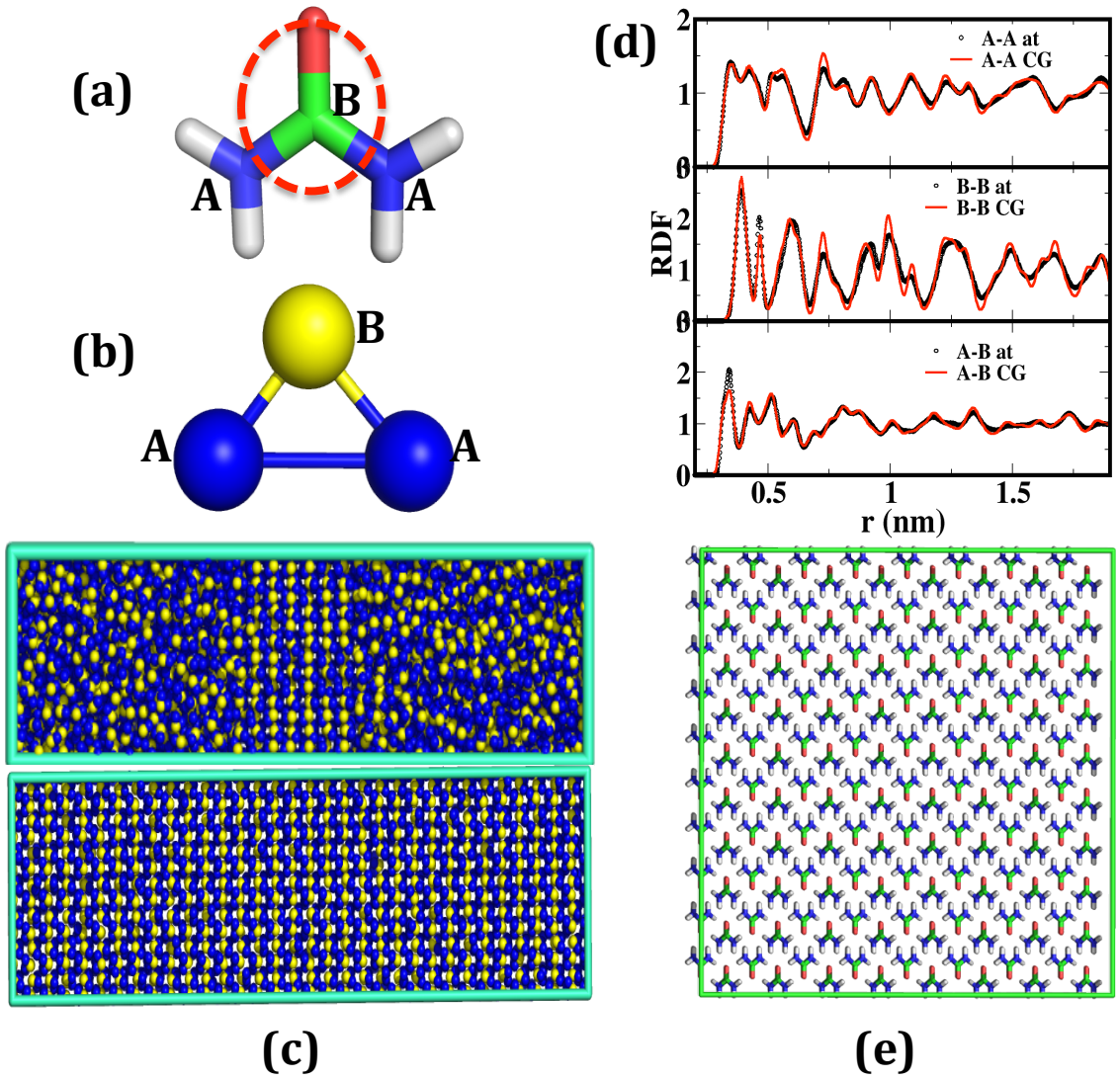

Figure S3: (a) atomistic representation of the urea molecule (b) CG representation of the urea molecule (c) *upper panel*: initial configuration of the crystalline slab in between two molten layers *lower panel*: final configuration of the grown structure. (d) Comparison of the RDFs of the CG beads with atomistic RDFs for the crystal structure grown from the melt. ‘at’ and ‘CG’ on the figure level stand for atomistic and coarse-grained, respectively. (e) Crystal structure of urea.

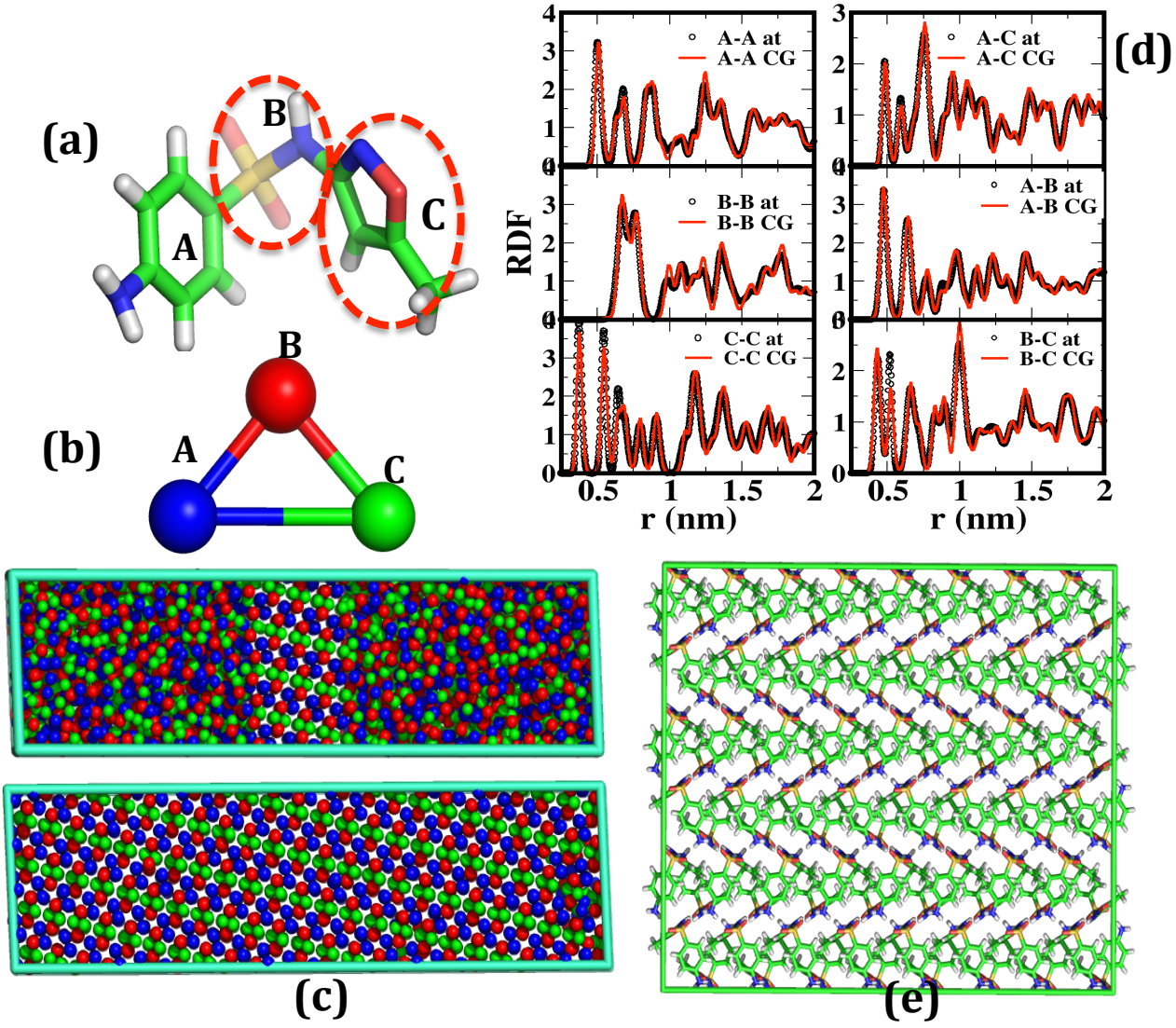

Figure S4: (a) atomistic representation of the sulfamethoxazole molecule (b) CG representation of the sulfamethoxazole molecule (c) *upper panel*: initial configuration of the crystalline slab in between two molten layers *lower panel*: final configuration of the grown structure. (d) Comparison of the RDFs of the CG beads with atomistic RDFs for the crystal structure grown from the melt. 'at' and 'CG' on the figure level stand for atomistic and coarse-grained, respectively. (e) Crystal structure of sulfamethoxazole.

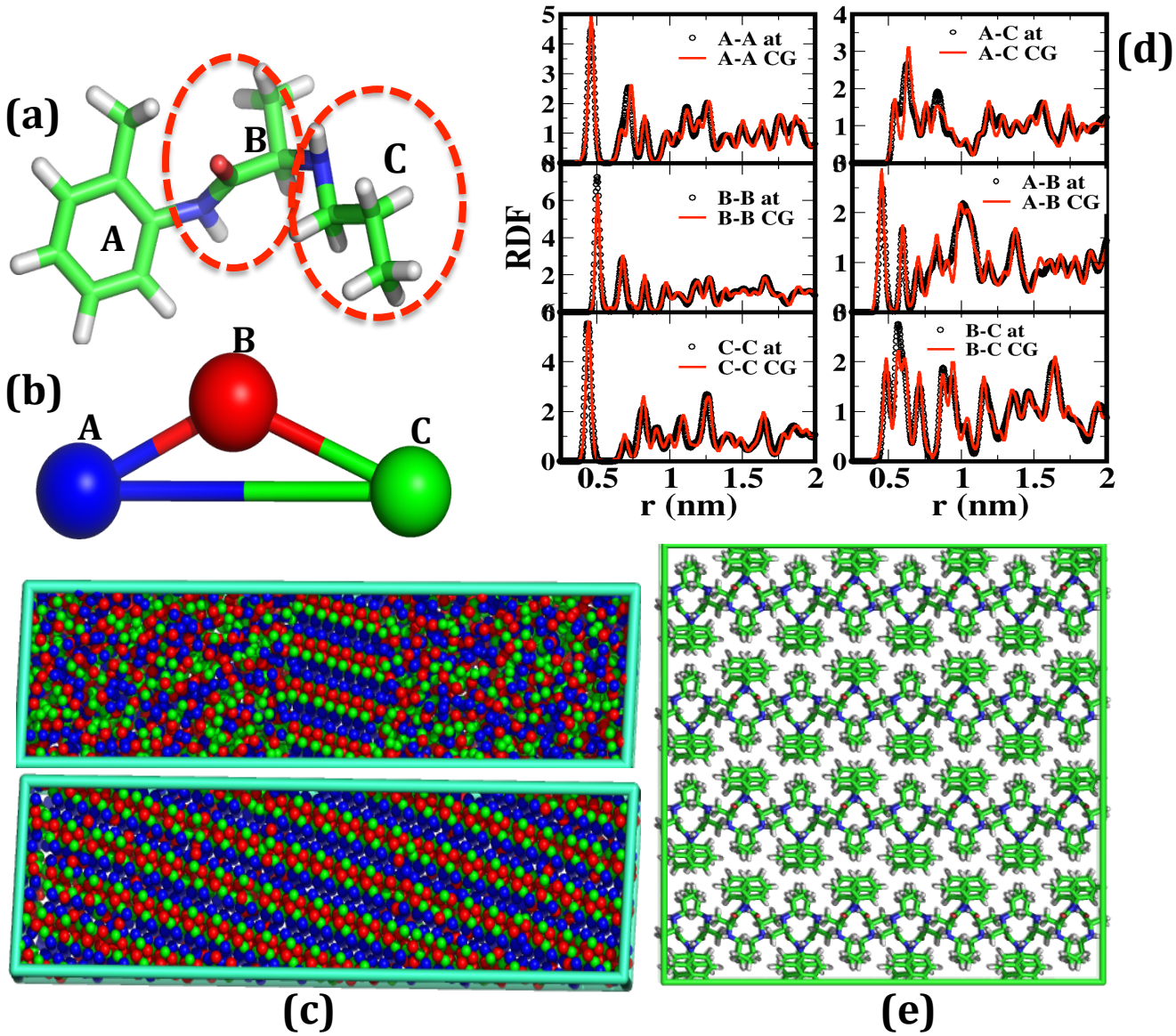

Figure S5: (a) atomistic representation of the prilocaine molecule (b) CG representation of the prilocaine molecule (c) *upper panel*: initial configuration of the crystalline slab in between two molten layers *lower panel*: final configuration of the grown structure. (d) Comparison of the RDFs of the CG beads with atomistic RDFs for the crystal structure grown from the melt. 'at' and 'CG' on the figure level stand for atomistic and coarse-grained, respectively. (e) Crystal structure of prilocaine.

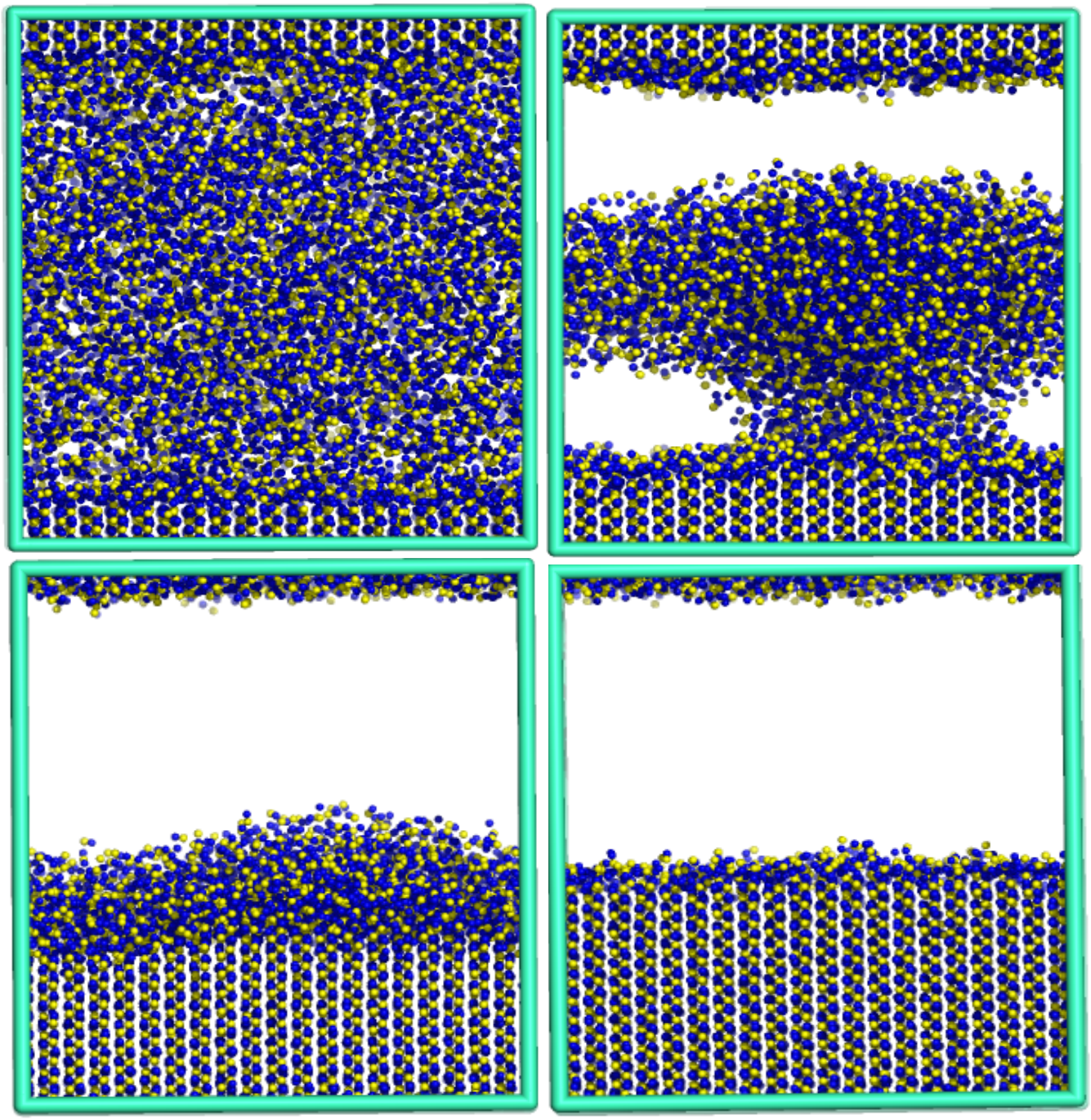

Figure S6: Snapshots of the drug molecules in the absence of polymers after 0 ns (top left panel), 6 ns (top right panel), 15 ns (bottom left panel) and 40 ns (bottom right panel)

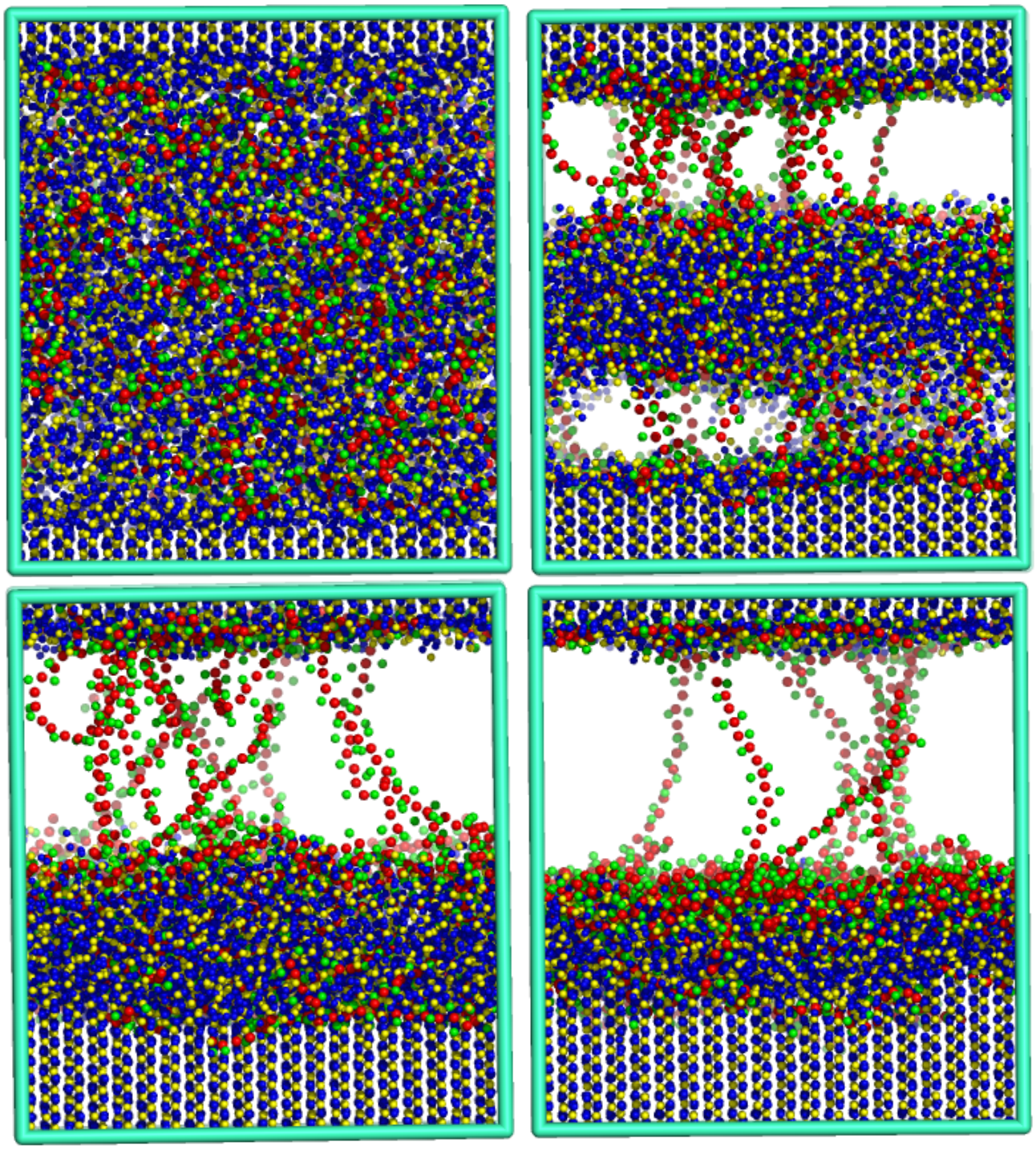

Figure S7: Snapshots of the drug molecules (blue and yellow) in the presence of 26Me3Su polymers (red and green) after 0 ns (top left panel), 25 ns (top right panel), 50 ns (bottom left panel) and 145 ns (bottom right panel).

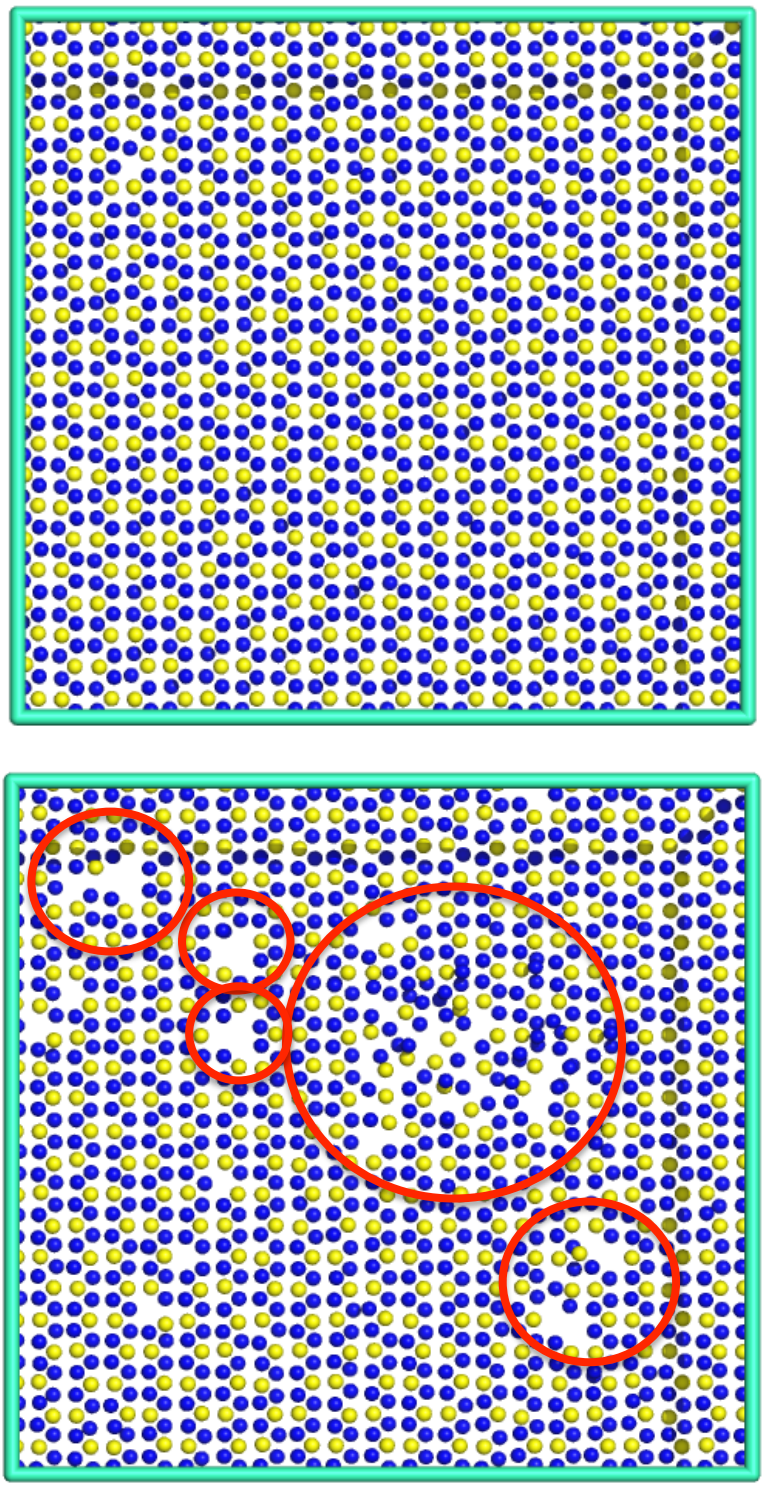

Figure S8: *Upper panel*: Snapshots of a perfect crystal layer grown in the absence of polymers. *Lower panel:* snapshots of a defect-containing crystal layer grown in the presence of 26Me3Su polymers.

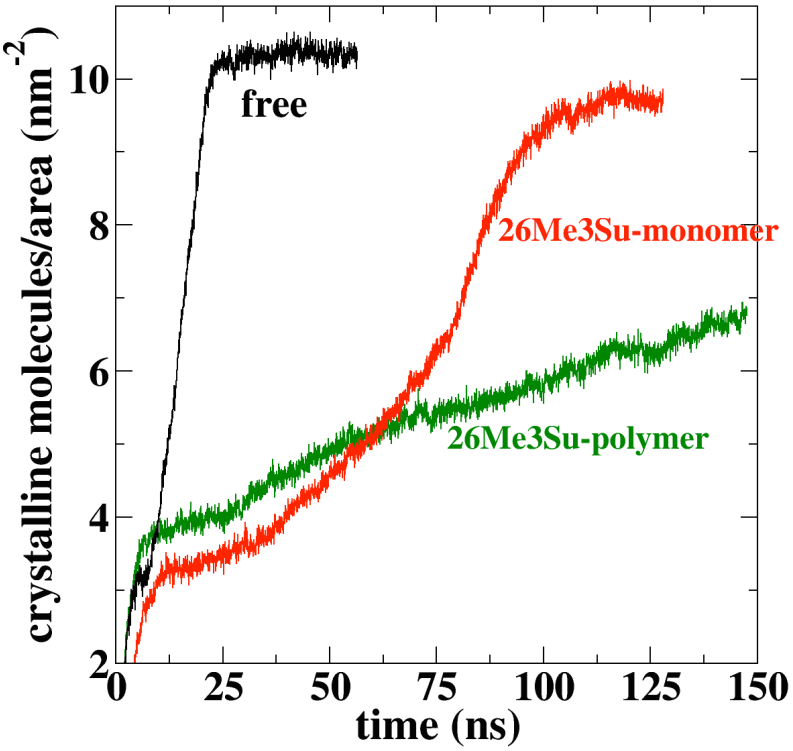

Figure S9: Crystal growth profile of phenytoin in the presence of 26Me3Su polymers and 26Me3Su monomers. ‘Free’ represents the system with no polymer or monomer.