Journal Name

ARTICLE

Electronic Supplementary Information for:

Molecular Dynamics Simulations Reveal Disruptive Self-Assembly in Dynamic Peptide Libraries

Received 00th January 20xx,
Accepted 00th January 20xx

DOI: 10.1039/x0xx00000x

www.rsc.org/

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Electronic Supplementary Information (ESI) available: Extra simulation snapshots. See DOI: 10.1039/x0xx00000x

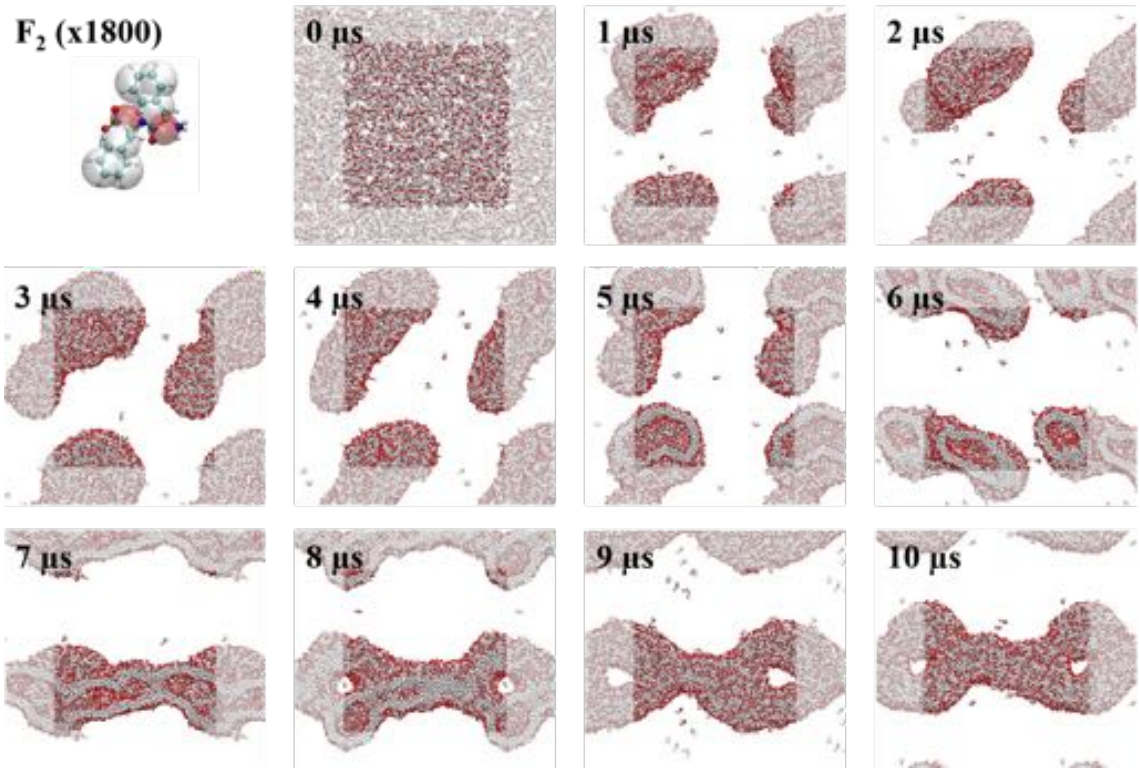

Figure S1. F_2 atomistic to CG representation and CG simulation snapshots every microsecond. System composed of 1800 molecules with backbone beads in red and side chain beads in white. Water removed for clarity.

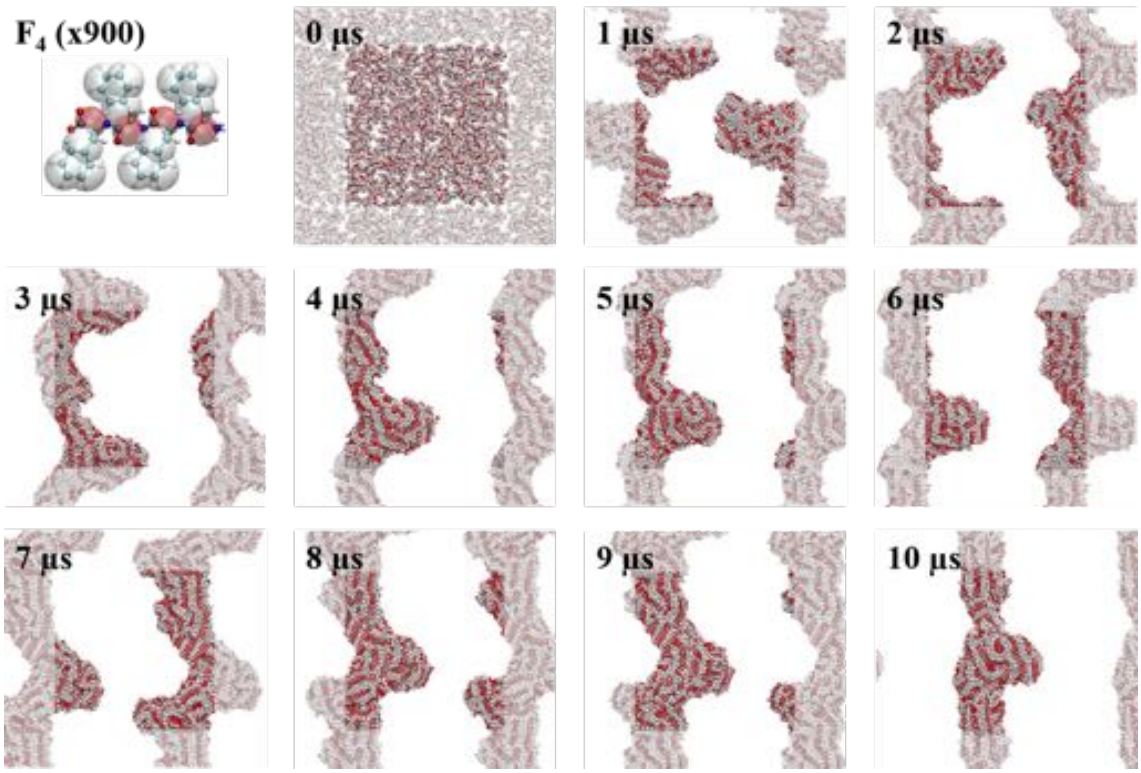

Figure S2. F_4 atomistic to CG representation and CG simulation snapshots every microsecond. System composed of 900 molecules with backbone beads in red and side chain beads in white. Water removed for clarity.

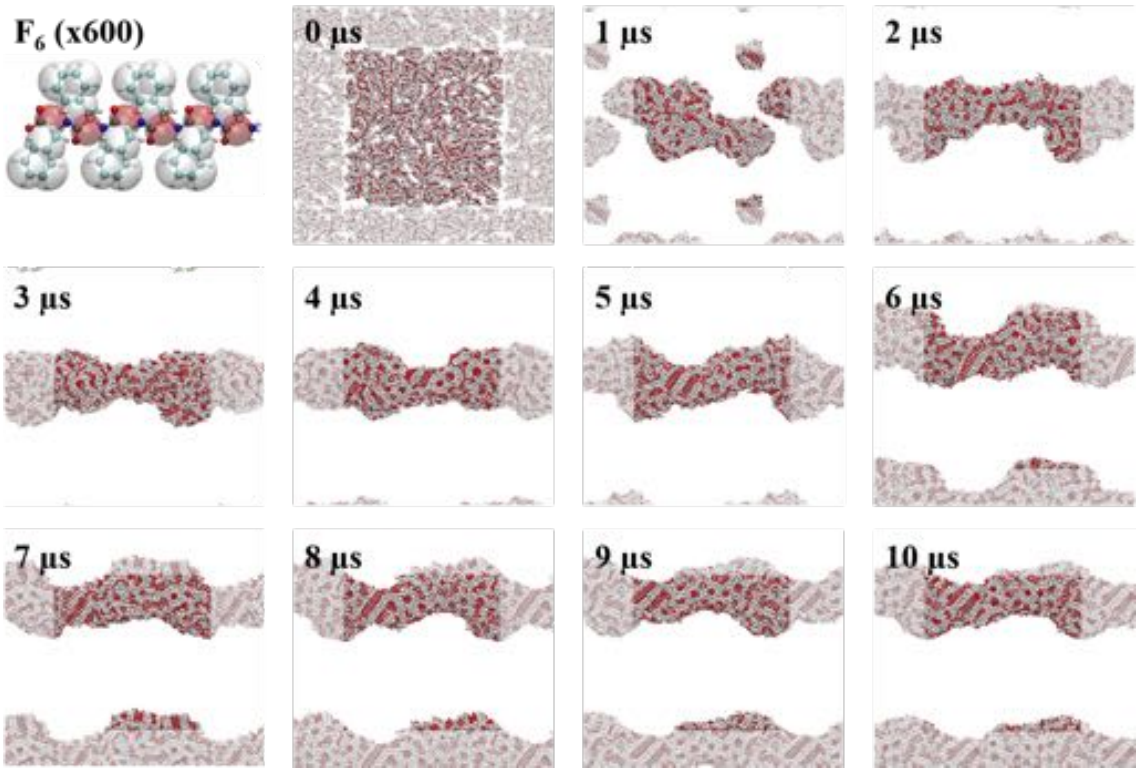

Figure S3. F_6 atomistic to CG representation and CG simulation snapshots every microsecond. System composed of 600 molecules with backbone beads in red and side chain beads in white. Water removed for clarity.

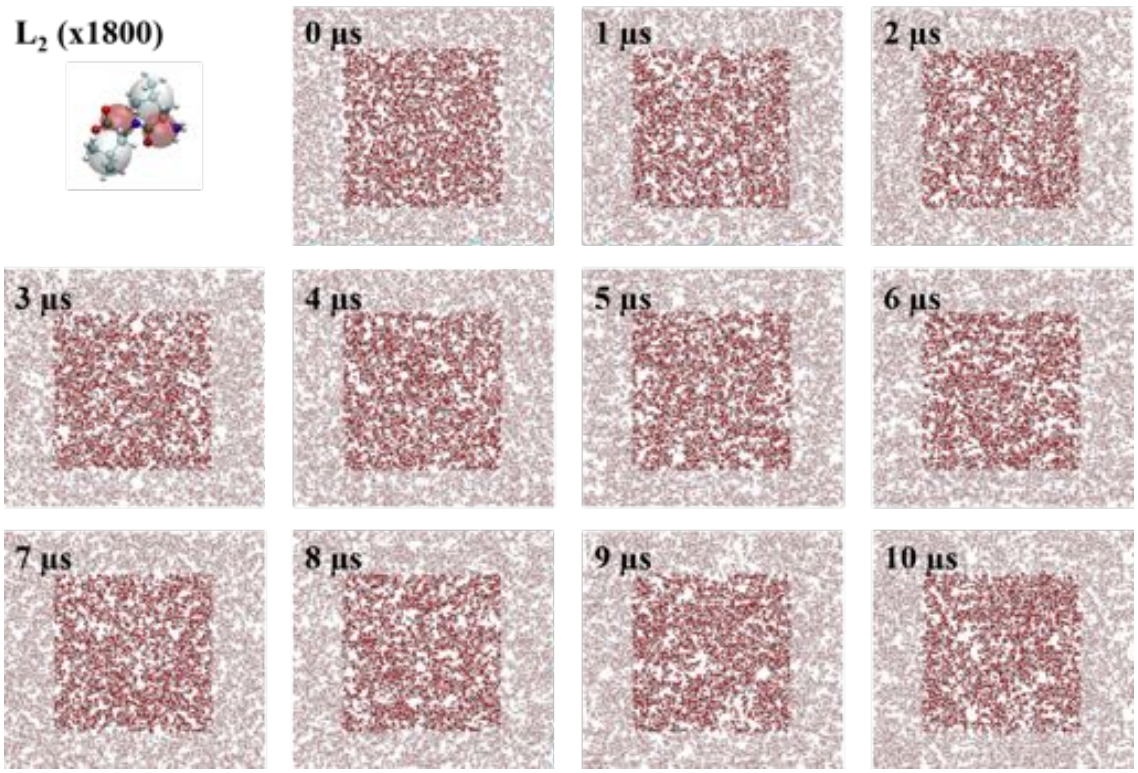

Figure S4. L_2 atomistic to CG representation and CG simulation snapshots every microsecond. System composed of 1800 molecules with backbone beads in red and side chain beads in white. Water removed for clarity.

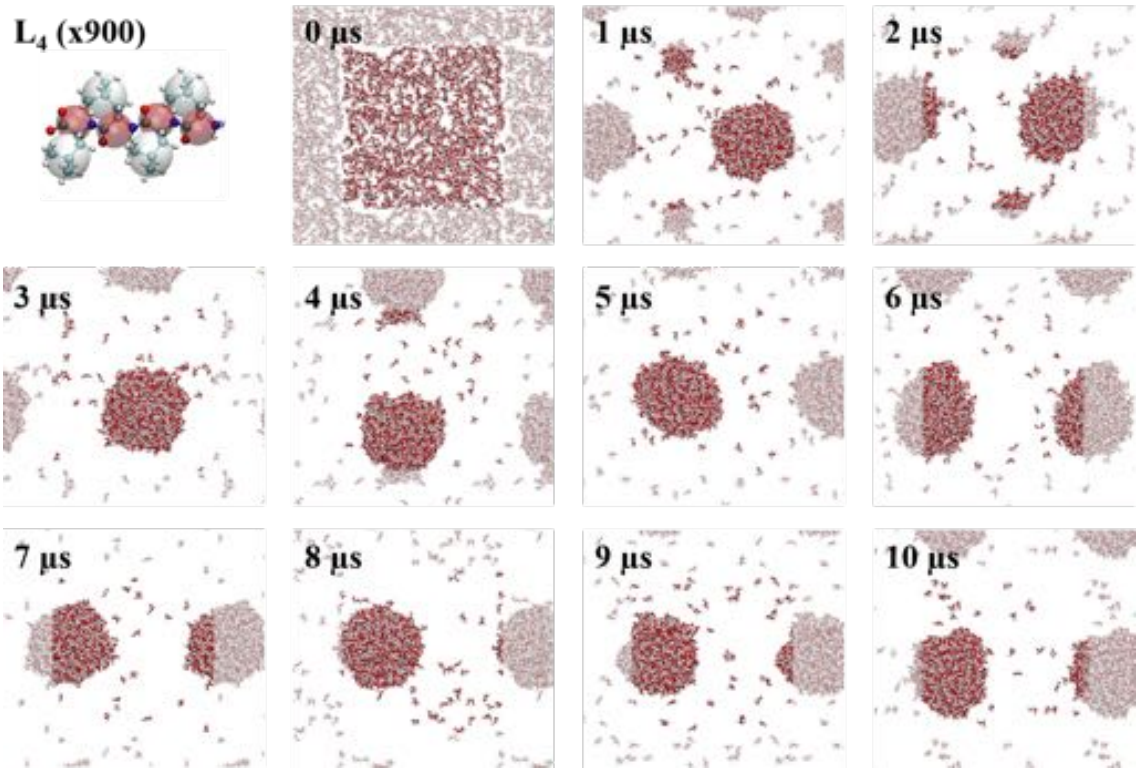

Figure S5. L_4 atomistic to CG representation and CG simulation snapshots every microsecond. System composed of 900 molecules with backbone beads in red and side chain beads in white. Water removed for clarity.

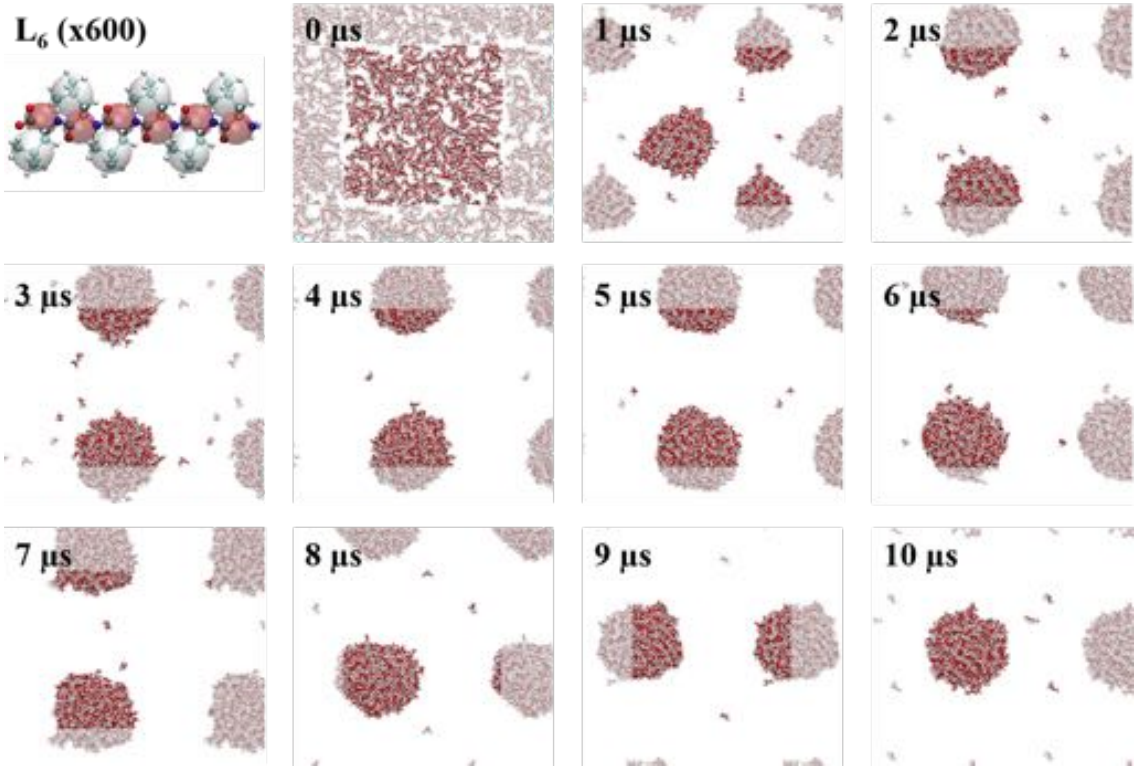

Figure S6. L_6 atomistic to CG representation and CG simulation snapshots every microsecond. System composed of 600 molecules with backbone beads in red and side chain beads in white. Water removed for clarity.

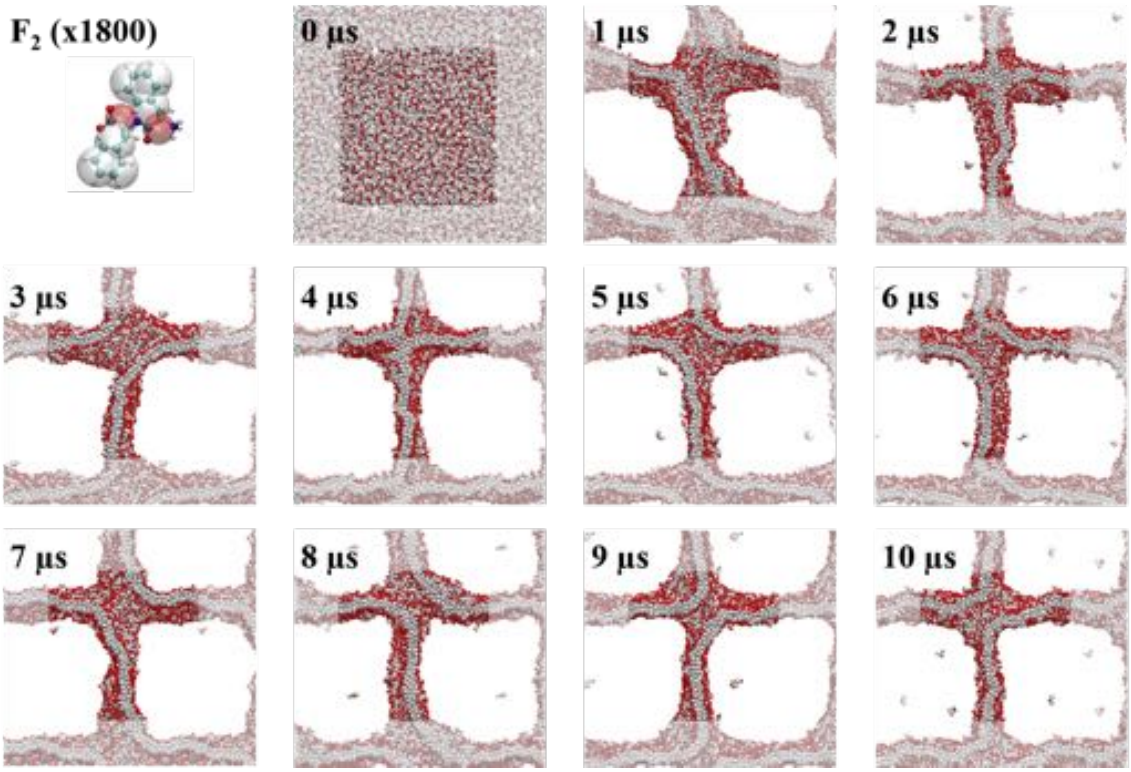

Figure S7. F_2 atomistic to CG representation and snapshots of the concentrated (half volume than in Figure S1) CG simulation, every microsecond from top view. System composed of 1800 molecules with backbone beads in red and side chain beads in white. Water removed for clarity.

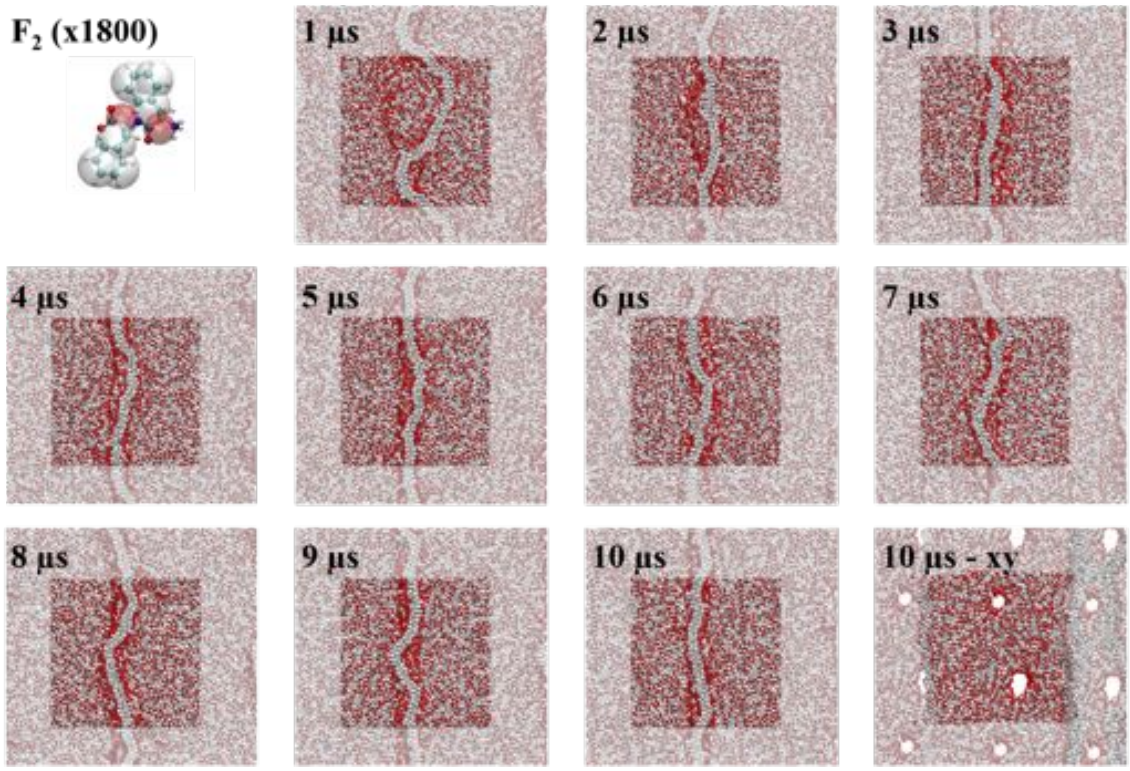

Figure S8. F_2 atomistic to CG representation and snapshots of the concentrated (half volume than in Figure S1) CG simulation, every microsecond from side view. System composed of 1800 molecules with backbone beads in red and side chain beads in white. *10 µs – xy* is taken from the *xy*-diagonal to show the holes in the junction of the two bilayers that can be seen in Figure S7. Water removed for clarity.

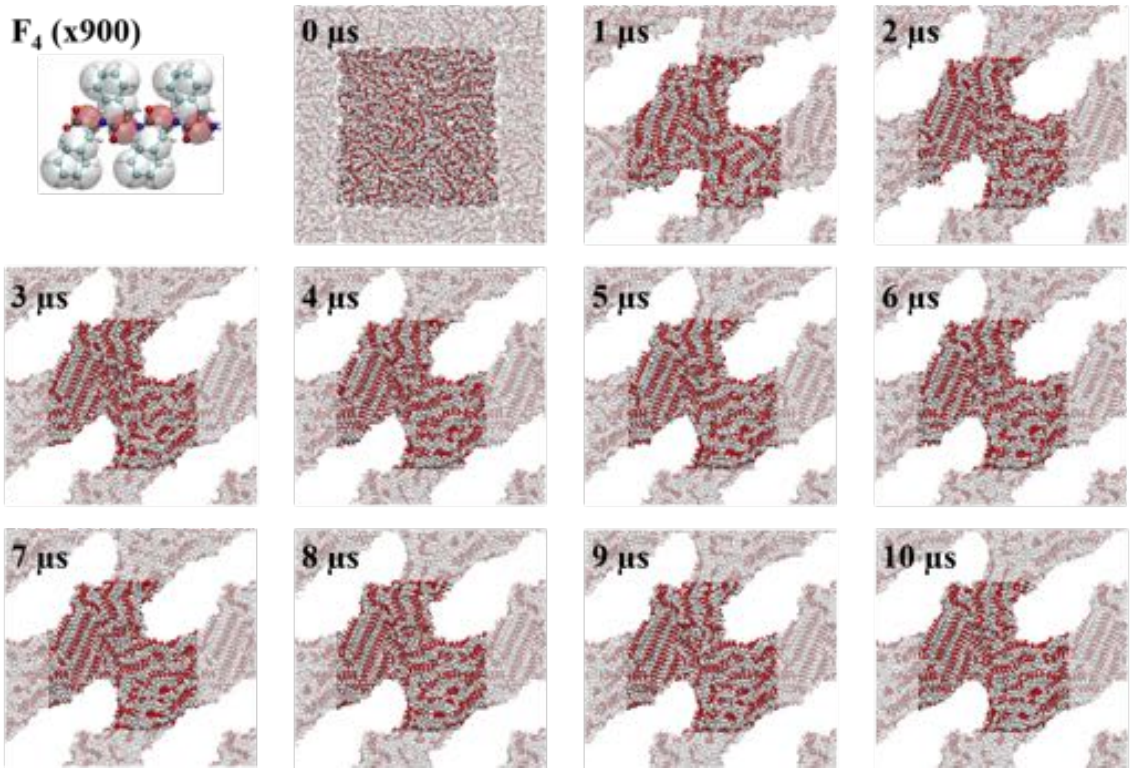

Figure S9. F_4 atomistic to CG representation and snapshots of the concentrated (half volume than in Figure S2) CG simulation, every microsecond. System composed of 900 molecules with backbone beads in red and side chain beads in white. Water removed for clarity.

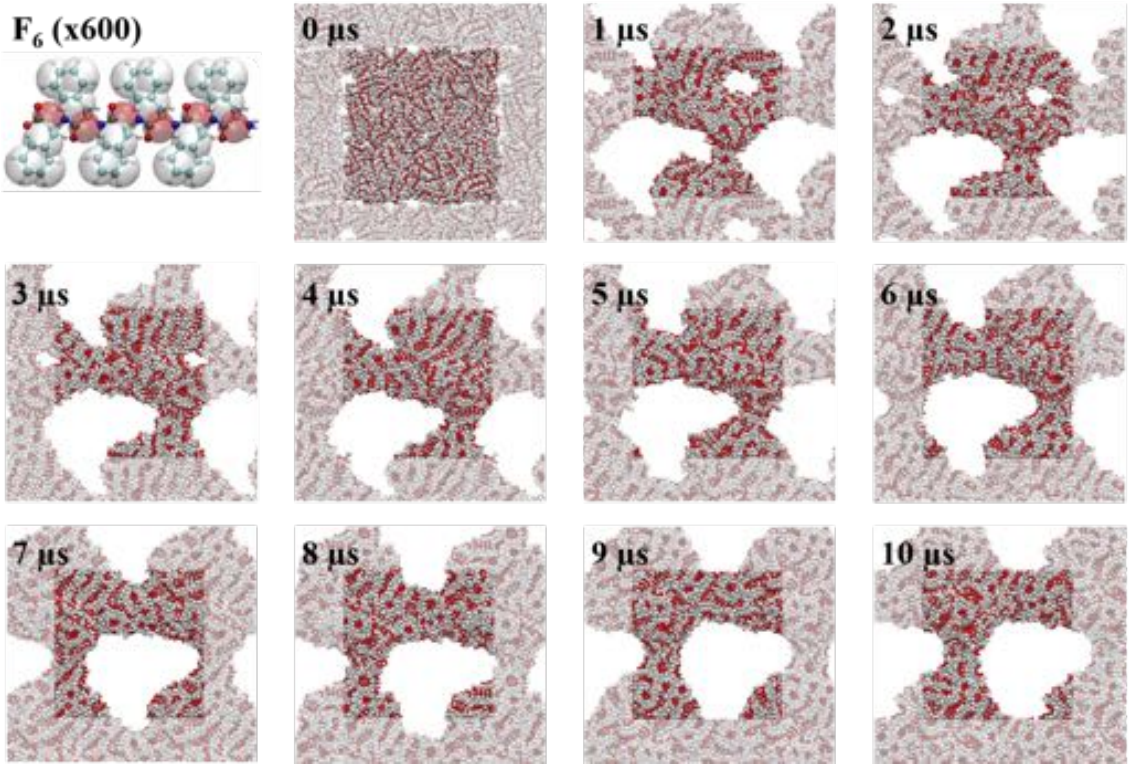

Figure S10. F_6 atomistic to CG representation and snapshots of the concentrated (half volume than in Figure S3) CG simulation, every microsecond. System composed of 600 molecules with backbone beads in red and side chain beads in white. Water removed for clarity.

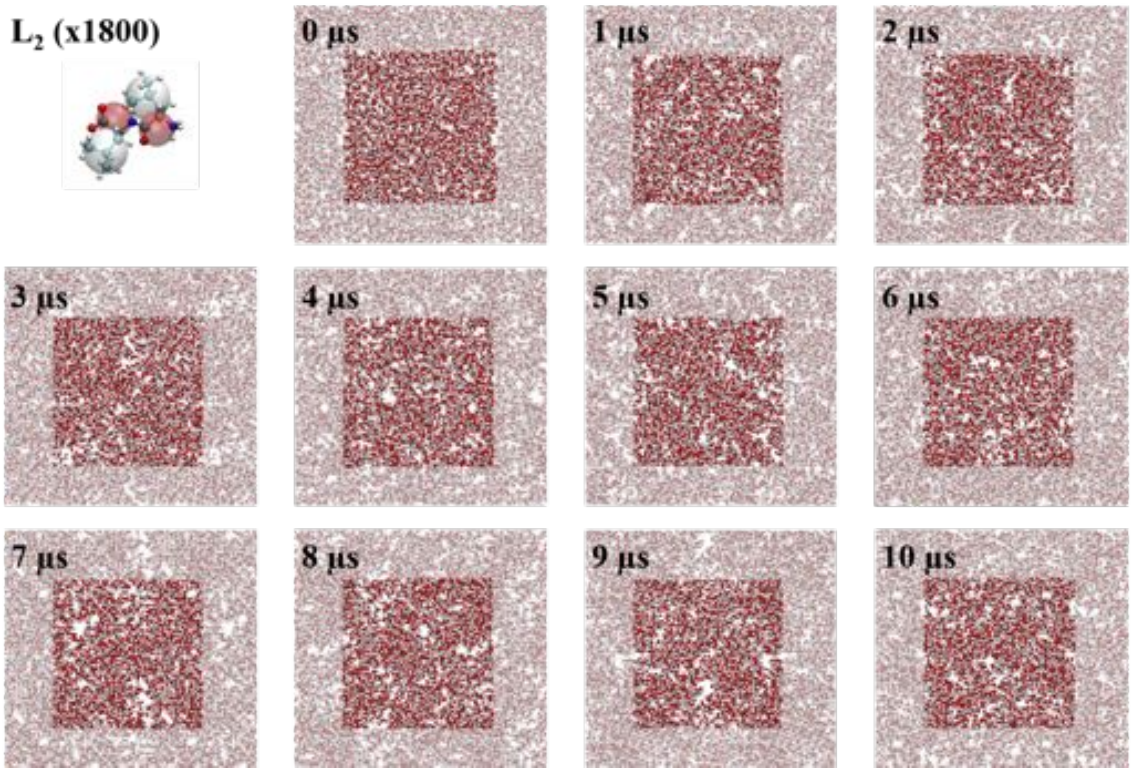

Figure S11. L_2 atomistic to CG representation and snapshots of the concentrated (half volume than in Figure S4) CG simulation, every microsecond. System composed of 1800 molecules with backbone beads in red and side chain beads in white. Water removed for clarity.

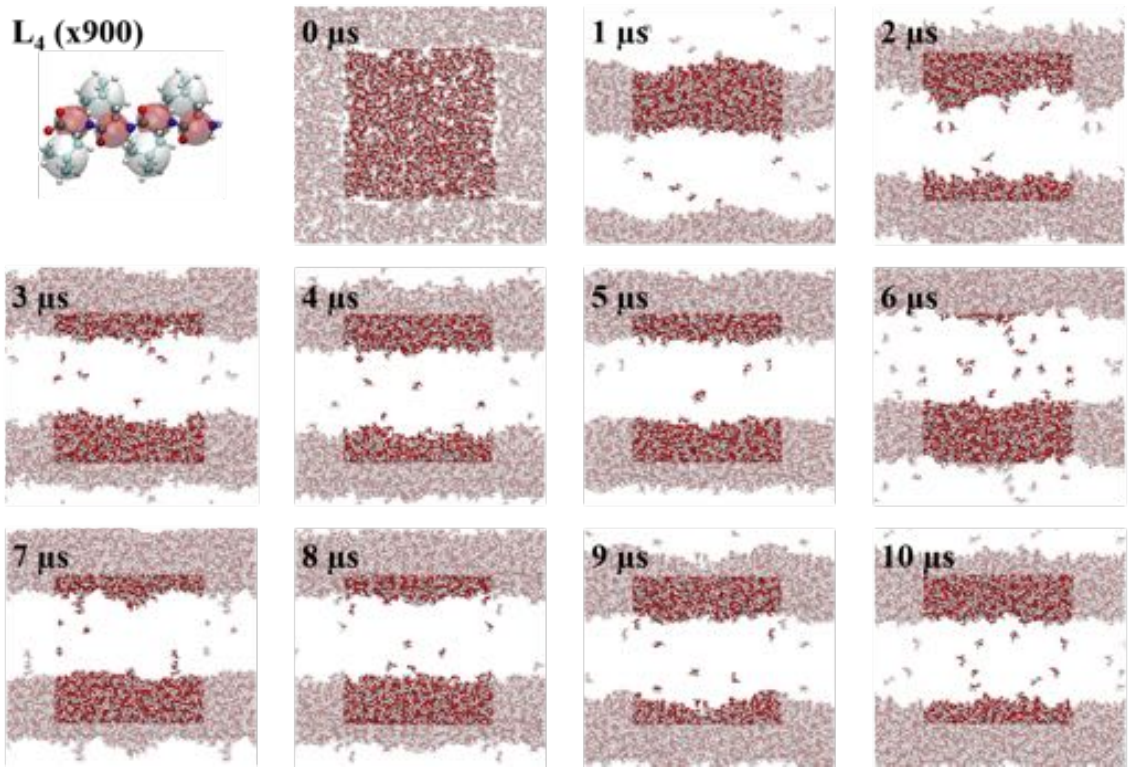

Figure S12. L_4 atomistic to CG representation and snapshots of the concentrated (half volume than in Figure S5) CG simulation, every microsecond. System composed of 900 molecules with backbone beads in red and side chain beads in white. Water removed for clarity.

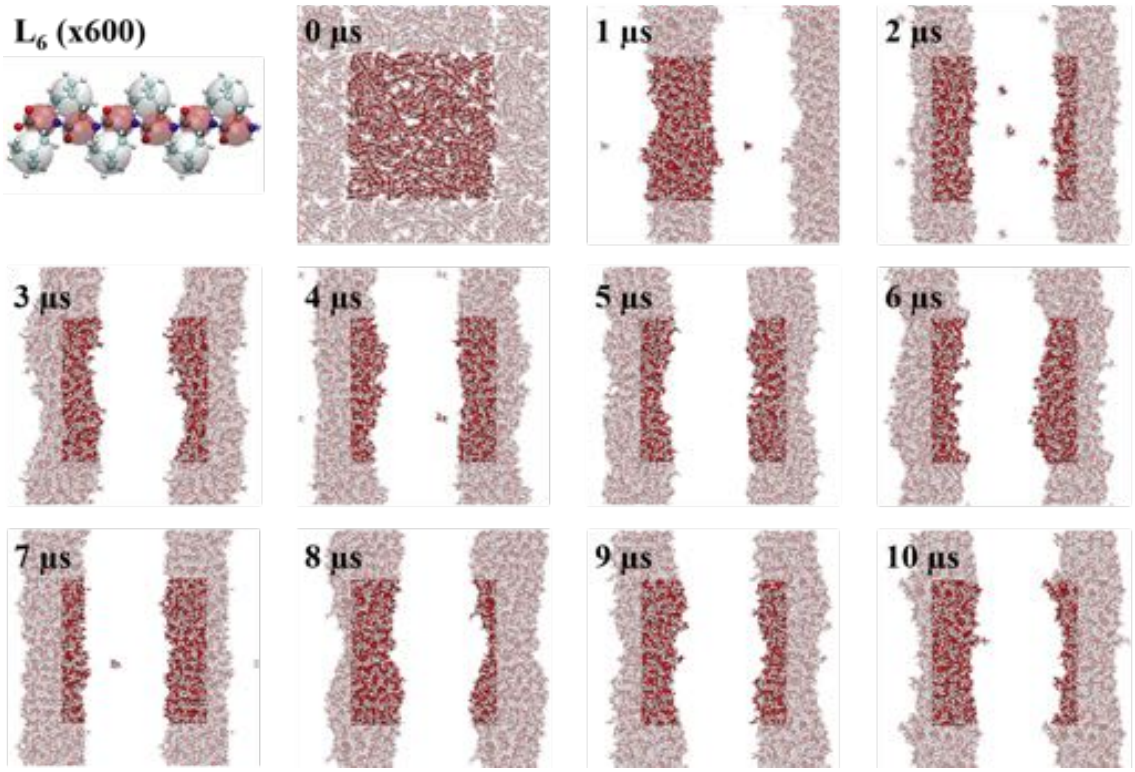

Figure S13. L_6 atomistic to CG representation and snapshots of the concentrated (half volume than in Figure S6) CG simulation, every microsecond. System composed of 600 molecules with backbone beads in red and side chain beads in white. Water removed for clarity.

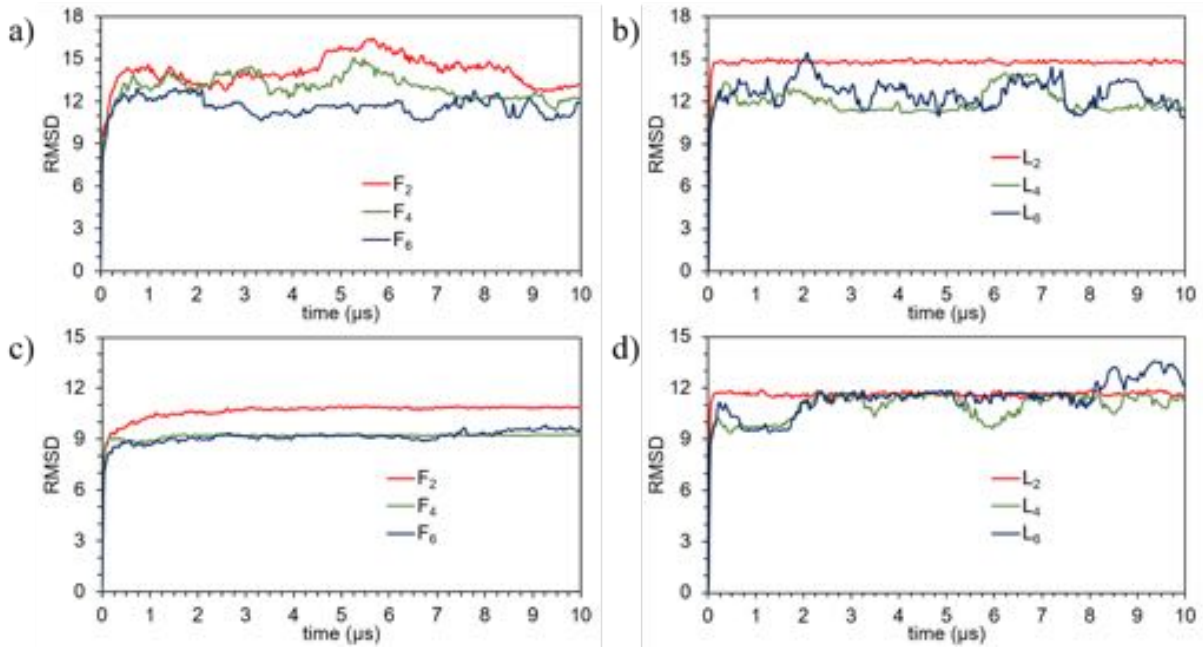

Figure S14. RMSD plots with time for (a-b) diluted systems and (c-d) concentrated systems for the F-peptides (a, c) and L-peptides (b, d).

The plots show the concentrated F systems (Fig. S14 c) to have low movement after 1 µs. F_6 shows slightly more fluctuations than F_2 and F_4. The L concentrated systems (Fig. S14b) show less fluctuations than the diluted (Fig. S14d), due to the nanostructure formation. L_2 shows negligible movement after 0.25 µs, but as the pictures show (Fig. S4 and S11) this is because of the averaged movement of the molecules in solution.

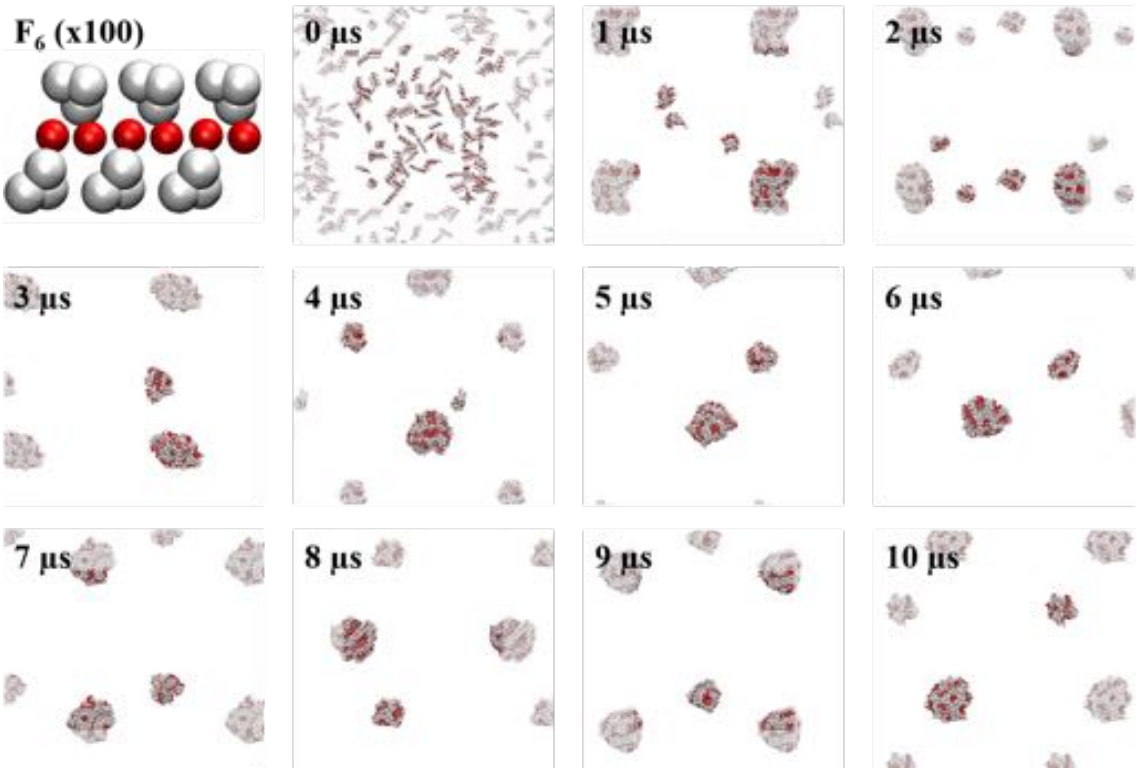

Figure S15. F_6 CG representation and F_6^{100} CG simulation snapshots every microsecond. System composed of 100 molecules with backbone beads in red and side chain beads in white. Water removed for clarity.

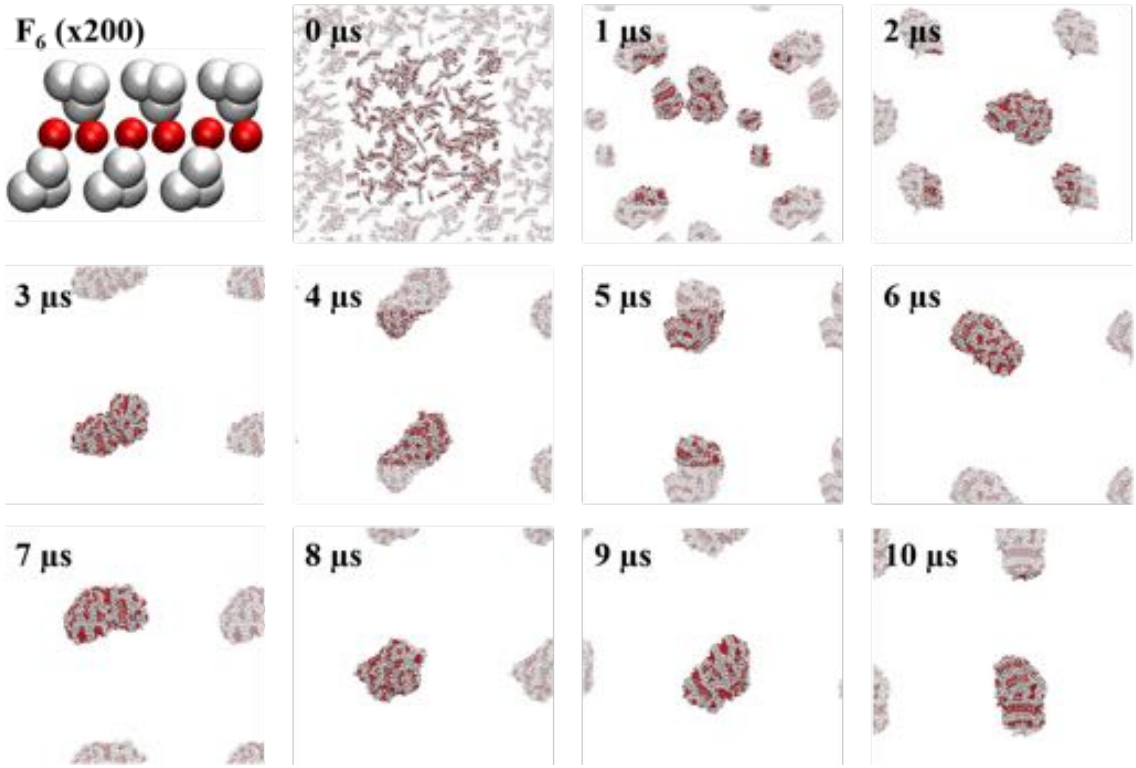

Figure S16. F_6 CG representation and F_6^{200} CG simulation snapshots every microsecond. System composed of 200 molecules with backbone beads in red and side chain beads in white. Water removed for clarity.

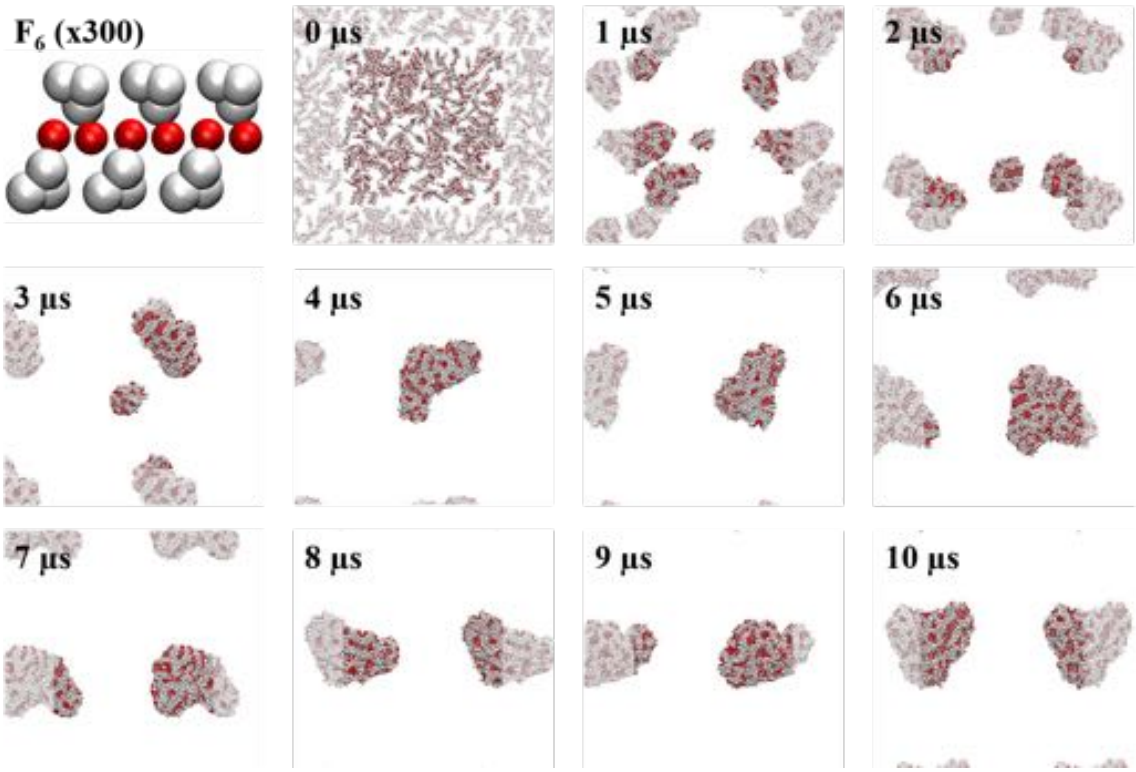

Figure S17. F_6 CG representation and F_6^{300} CG simulation snapshots every microsecond. System composed of 300 molecules with backbone beads in red and side chain beads in white. Water removed for clarity.

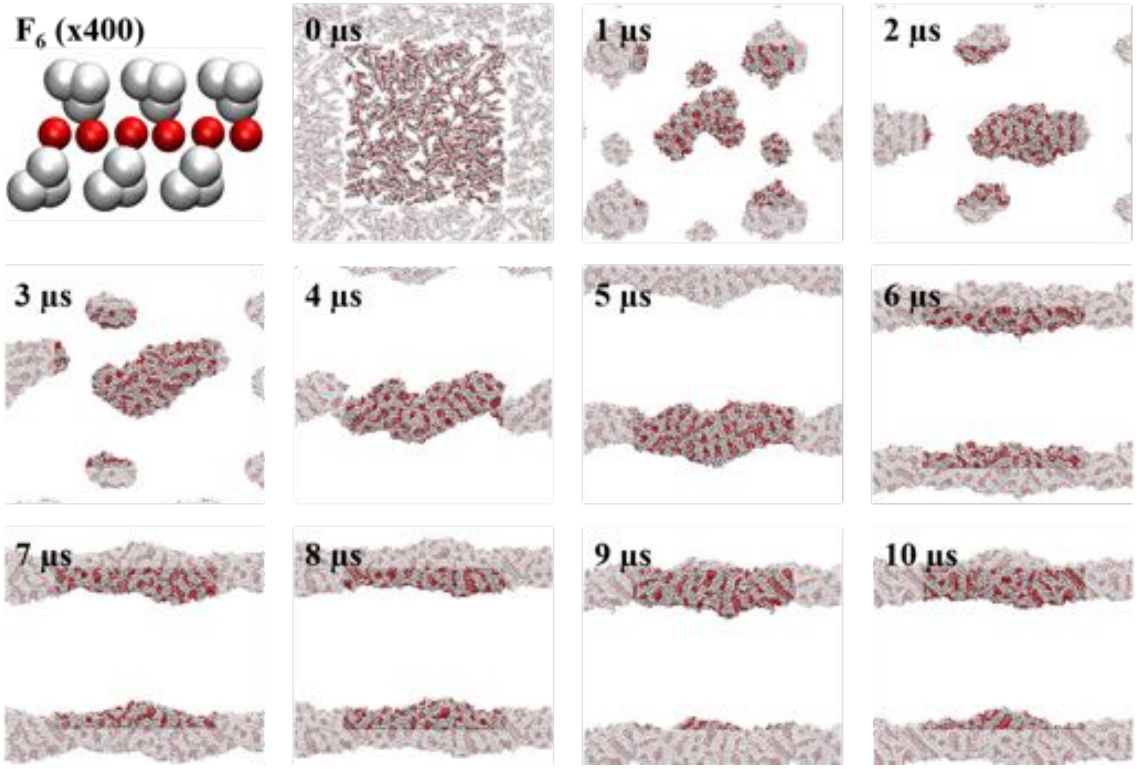

Figure S18. F_6 CG representation and F_6^{400} CG simulation snapshots every microsecond. System composed of 400 molecules with backbone beads in red and side chain beads in white. Water removed for clarity.

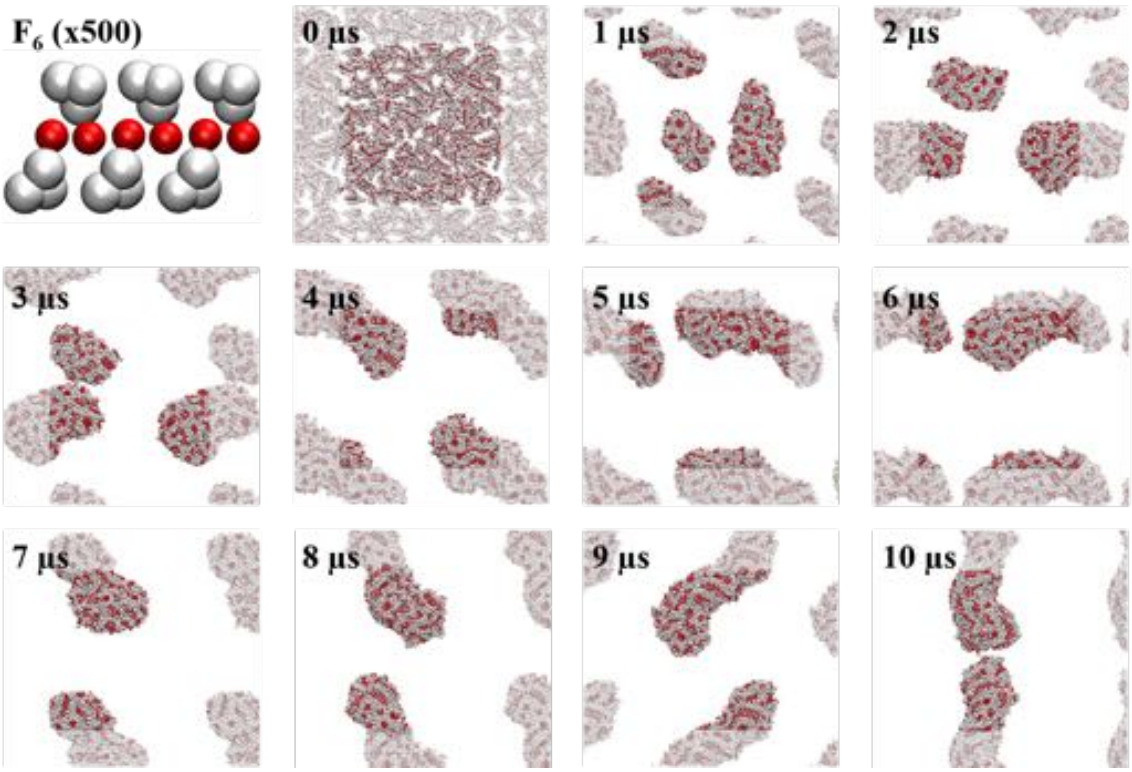

Figure S19. F_6 CG representation and F_6^{500} CG simulation snapshots every microsecond. System composed of 500 molecules with backbone beads in red and side chain beads in white. Water removed for clarity.

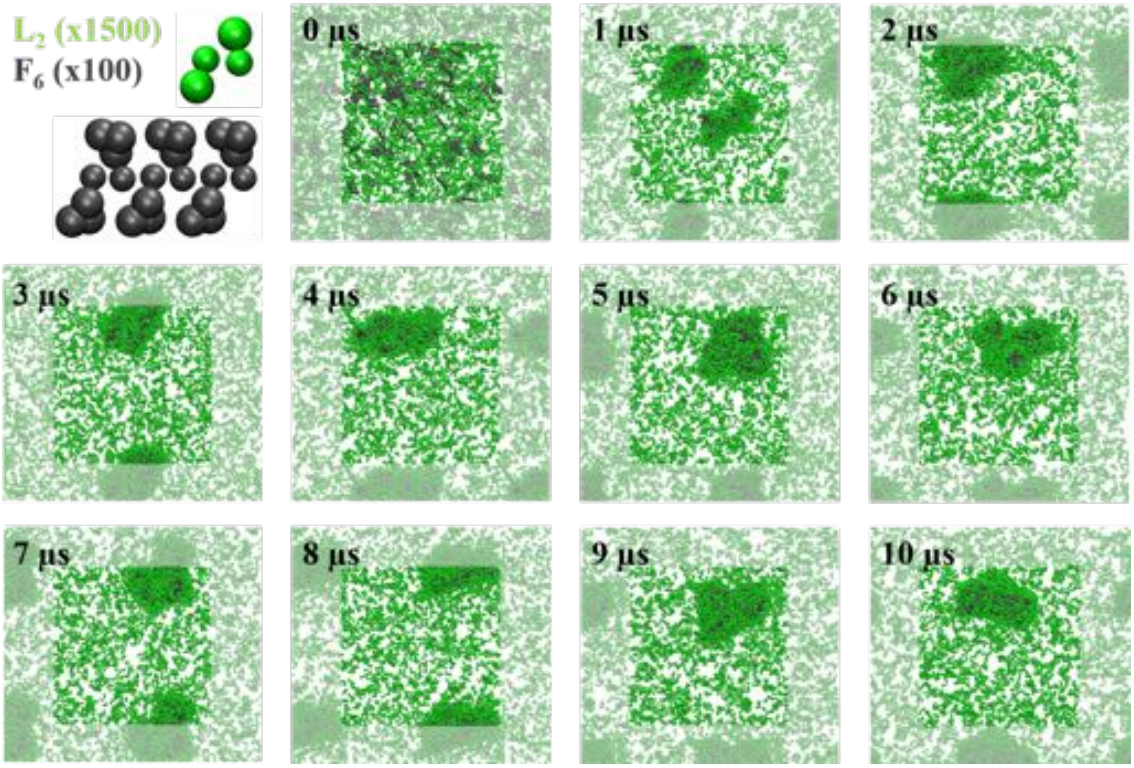

Figure S20. L_2 (green) and F_6 (grey) CG representations and $F\text{-}L^{100\text{-}1500}$ CG simulation snapshots every microsecond. System composed of 1500 L_2 molecules in green and 100 F_6 molecules in grey. Water removed for clarity.

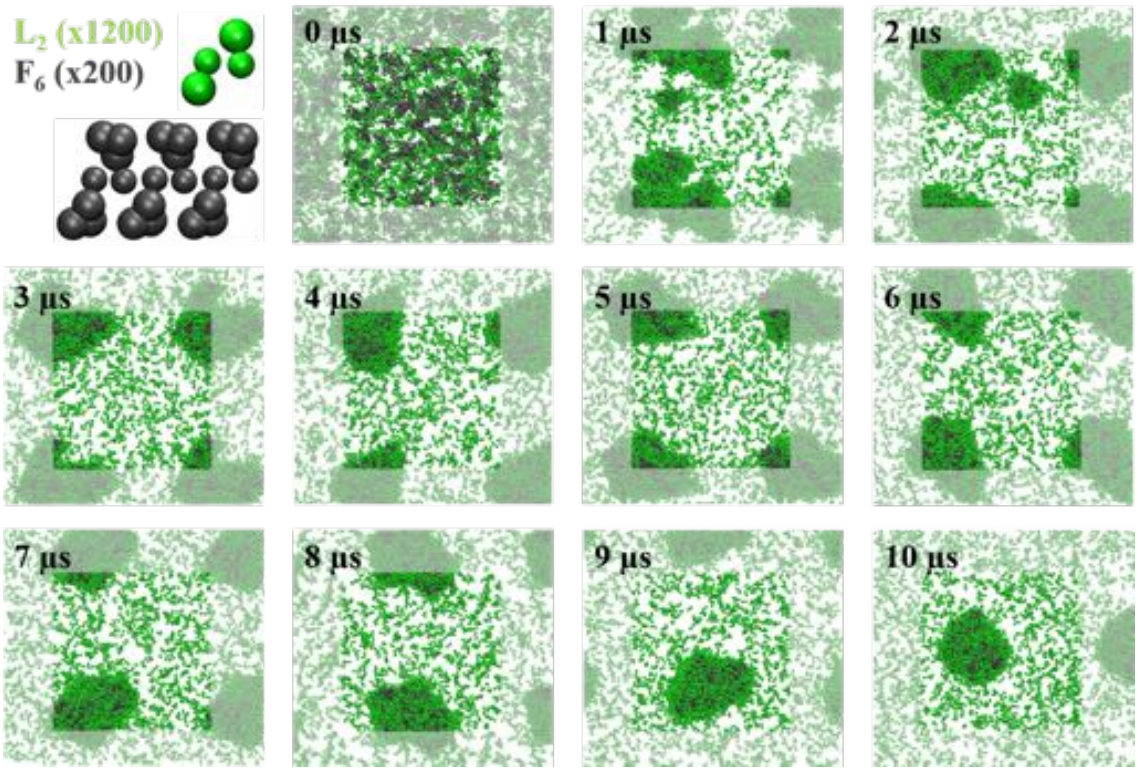

Figure S21. L_2 (green) and F_6 (grey) CG representations and *F-L*$^{200\text{-}1200}$ CG simulation snapshots every microsecond. System composed of 1200 L_2 molecules in green and 200 F_6 molecules in grey. Water removed for clarity.

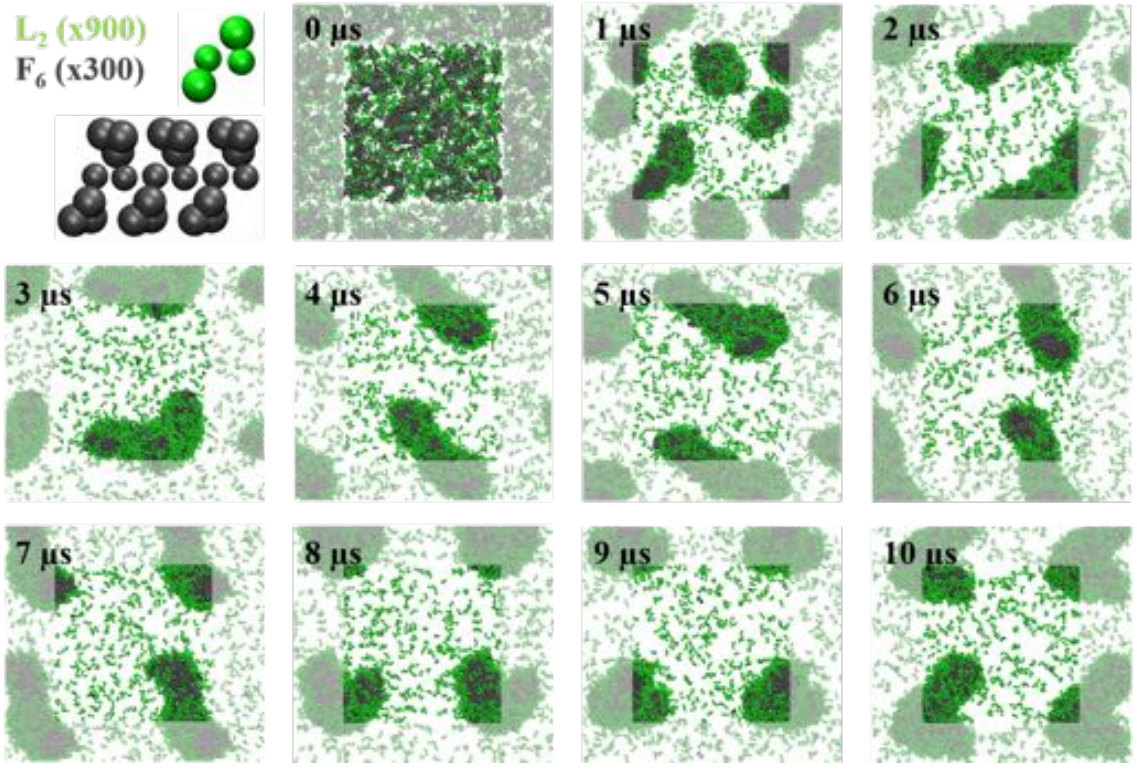

Figure S22. L_2 (green) and F_6 (grey) CG representations and *F-L*$^{300\text{-}900}$ CG simulation snapshots every microsecond. System composed of 900 L_2 molecules in green and 300 F_6 molecules in grey. Water removed for clarity.

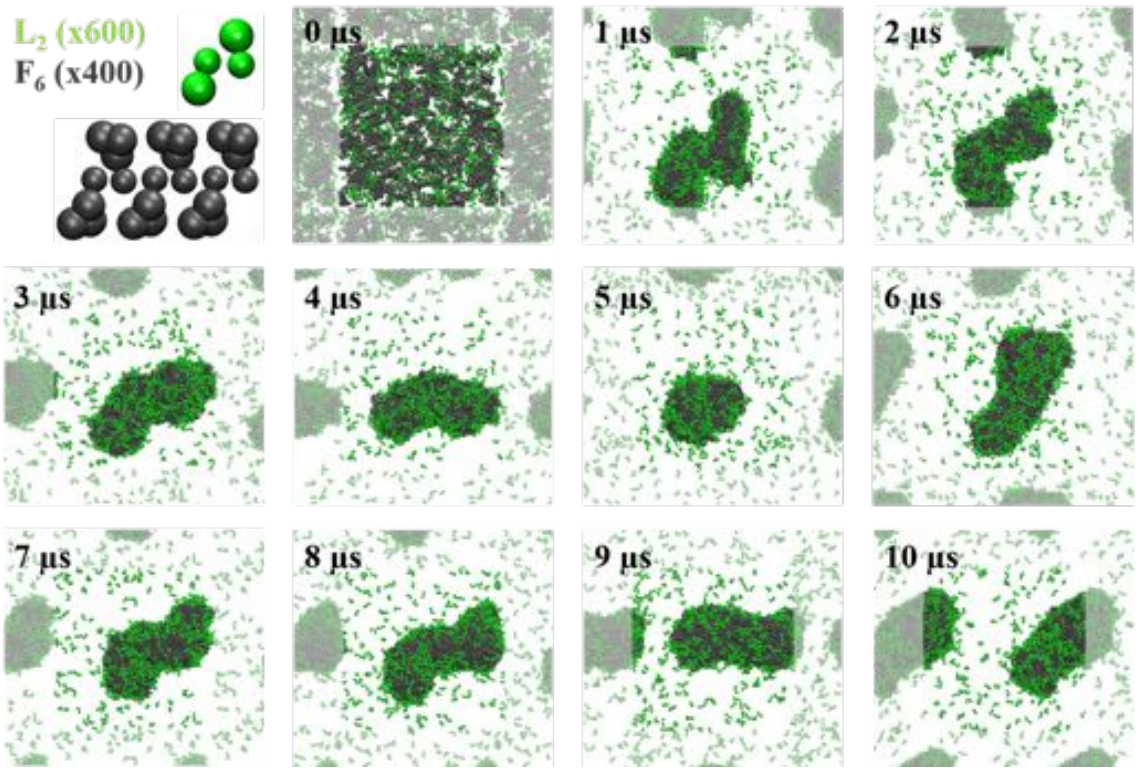

Figure S23. L_2 (green) and F_6 (grey) CG representations and *F-L*$^{400\text{-}600}$ CG simulation snapshots every microsecond. System composed of 600 L_2 molecules in green and 400 F_6 molecules in grey. Water removed for clarity.

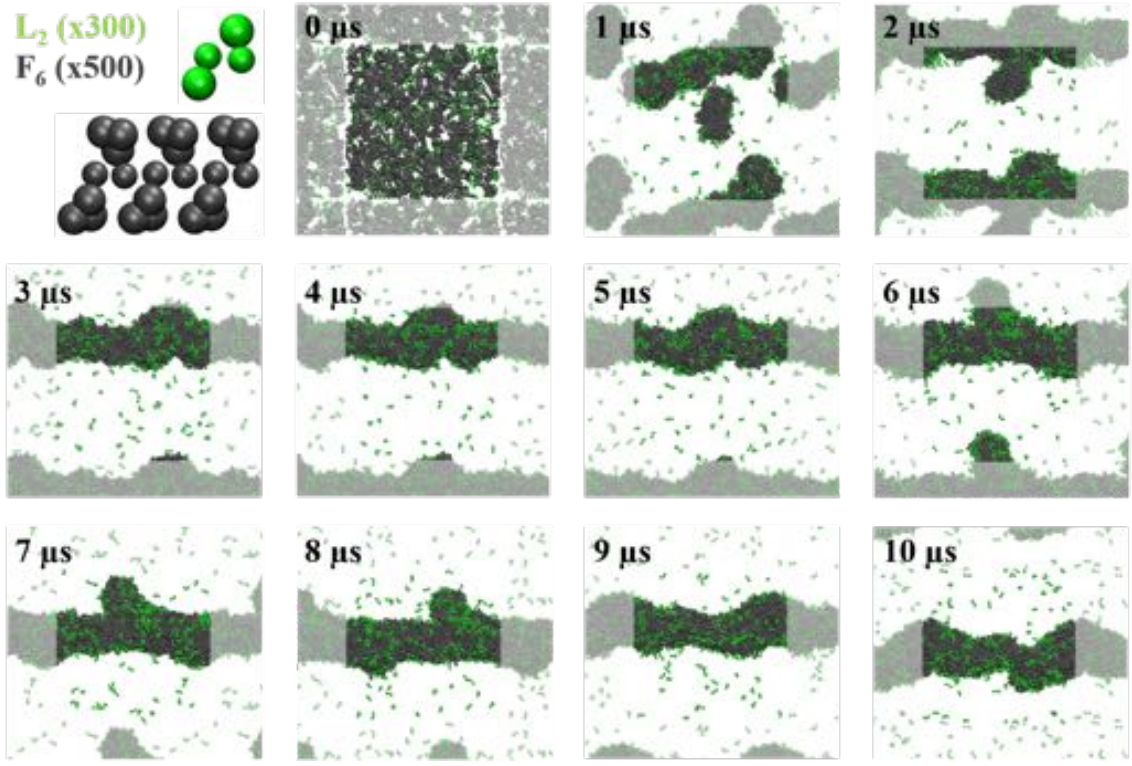

Figure S24. L_2 (green) and F_6 (grey) CG representations and *F-L*$^{500\text{-}300}$ CG simulation snapshots every microsecond. System composed of 300 L_2 molecules in green and 500 F_6 molecules in grey. Water removed for clarity.