

Supporting information for:

Directed Nano-scale Self-Assembly of Molecular Wires

Interconnecting Nodal Points

A. M. Boscoboinik¹, S. J. Manzi¹, W.T.Tysoe², V. D. Pereyra¹, J. A. Boscoboinik³

¹*Instituto de Fisica Aplicada INFAP-CONICET-Departamento de Fisica -Universidad Nacional de San Luis, Chacabuco 917-5700-San Luis, Argentina.*

²*Department of Chemistry and Biochemistry and Laboratory for Surface Studies, University of Wisconsin-Milwaukee, Milwaukee, Wisconsin 53211, United States.*

³*Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY 11973-5000, United States.*

In Figure S1, the assembly probability of the ECU₁₀ is plotted as a function of time (in MC steps) for various monomers coverages using a lattice with dimension $L = 40$. It can be seen in this plot that the system has already reached equilibrium after 10^5 MCs. This is similar to Figure 3 of the manuscript but extended to 10^7 MCs. Although we acknowledge that there are still small variations in PA when increasing the computational time by two orders of magnitude, the general conclusions of this work are not affected by these changes. Figure S2 shows a network of triangles. When connections are defined between the triangles, through their edges, a hexagonal network is formed. This concept is used in the manuscript to analyze the percolation of ECU's. Figures S3 to S7 show higher resolution versions of the snapshots shown in Figures 7 for the simulation of the formation of the network of triangles. Snapshots 1 to 3 (Figs S3 to S5) correspond to coverages above the percolation threshold. Snapshots 4 and 5 (Figs S6 and S7) correspond to coverages below and above the percolation threshold respectively.

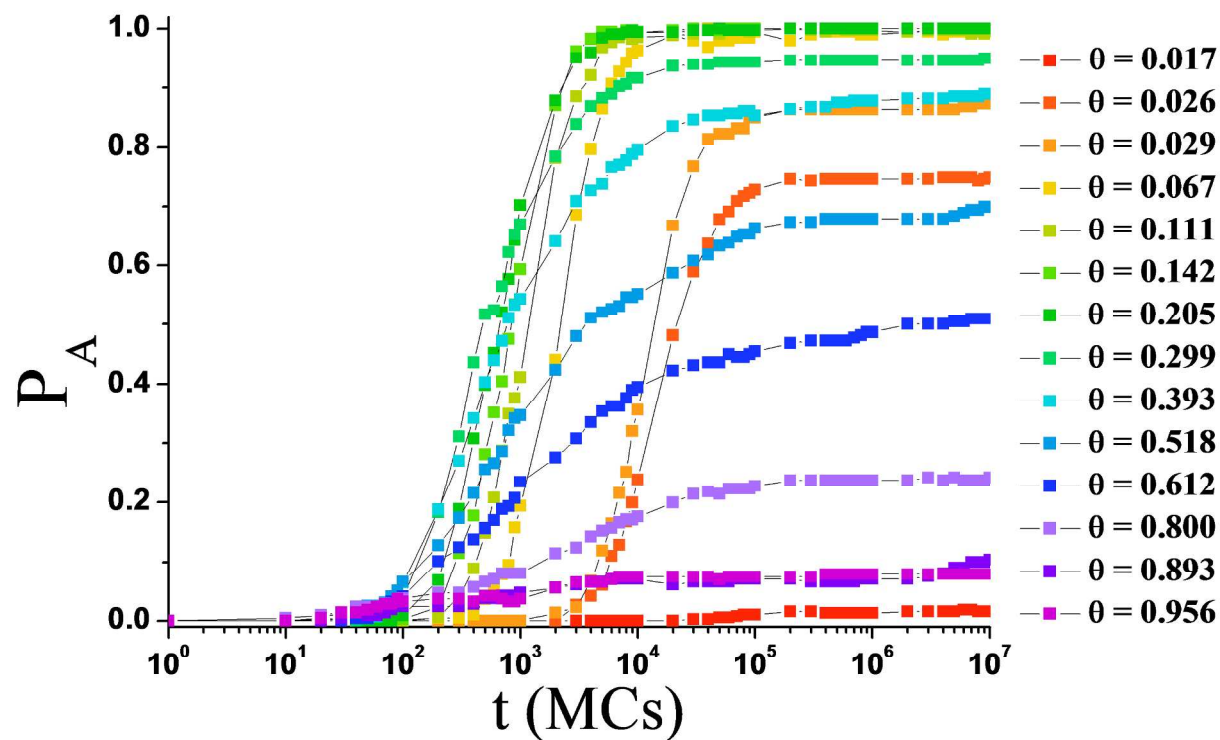


Fig. S1. Assembly probability (P_A) of an ECU as a function of time (MCs), for different coverages, for a lattice of size $L = 40$, with a nodal distance “ m ” = 10 and an interaction “ w ” = 124 kJ/mol.

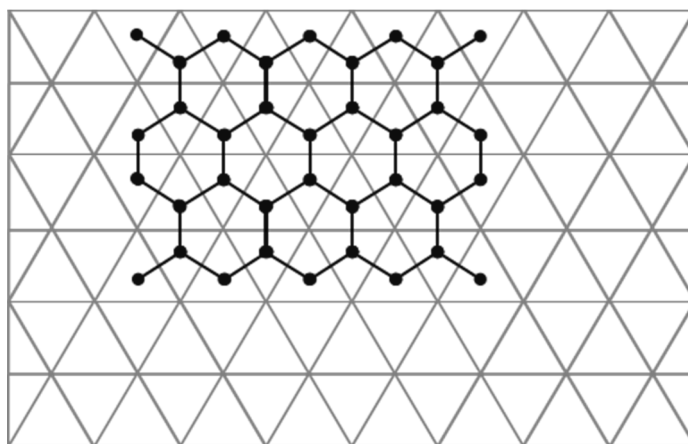


Fig. S2. Network of triangles connected by the edges. The interconnections form a hexagonal lattice.

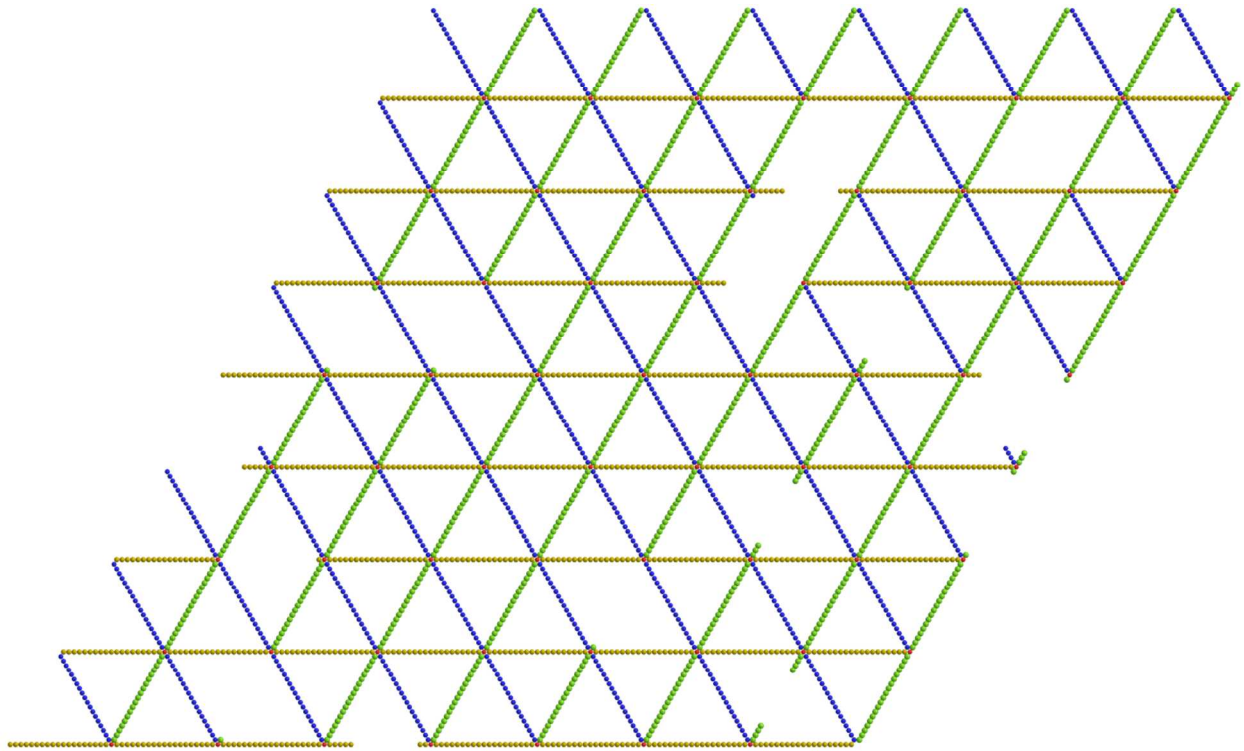


Fig. S3. Snapshot at $\theta = 0.13$, corresponding to inset 1 in Fig. 7 of the manuscript.

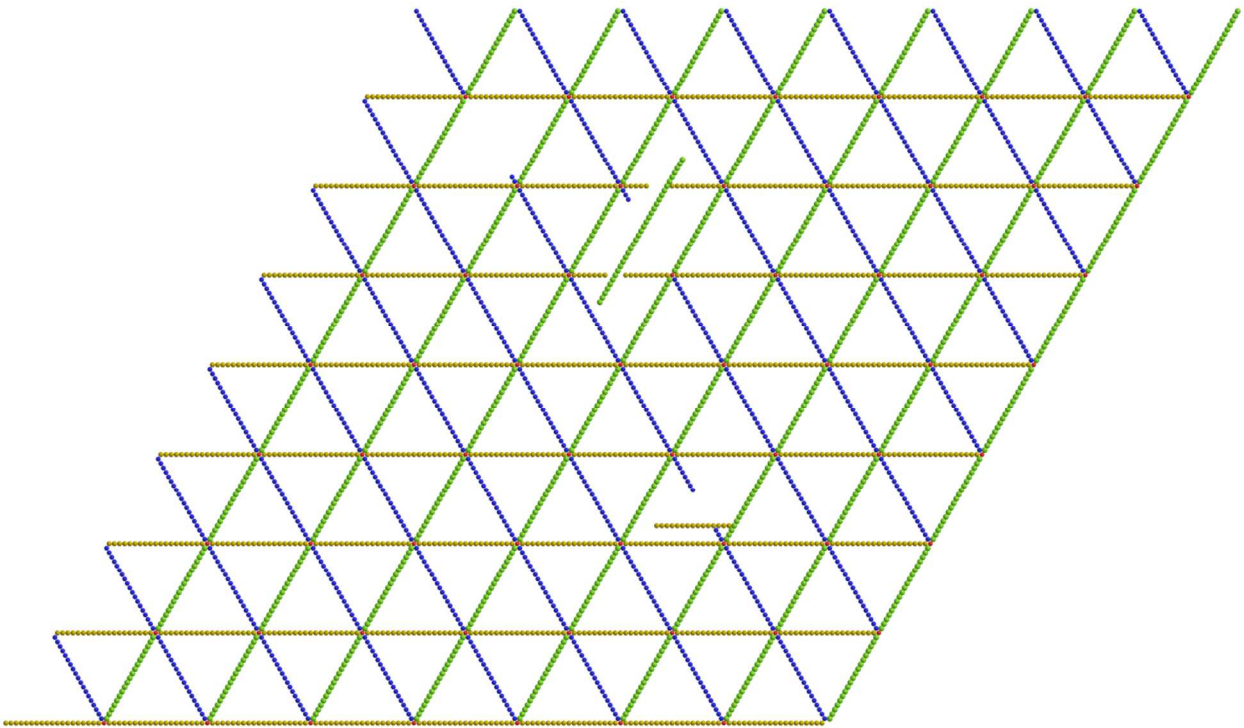


Fig. S4. Snapshot at $\theta = 0.14$, corresponding to inset 2 in Fig. 7 of the manuscript.

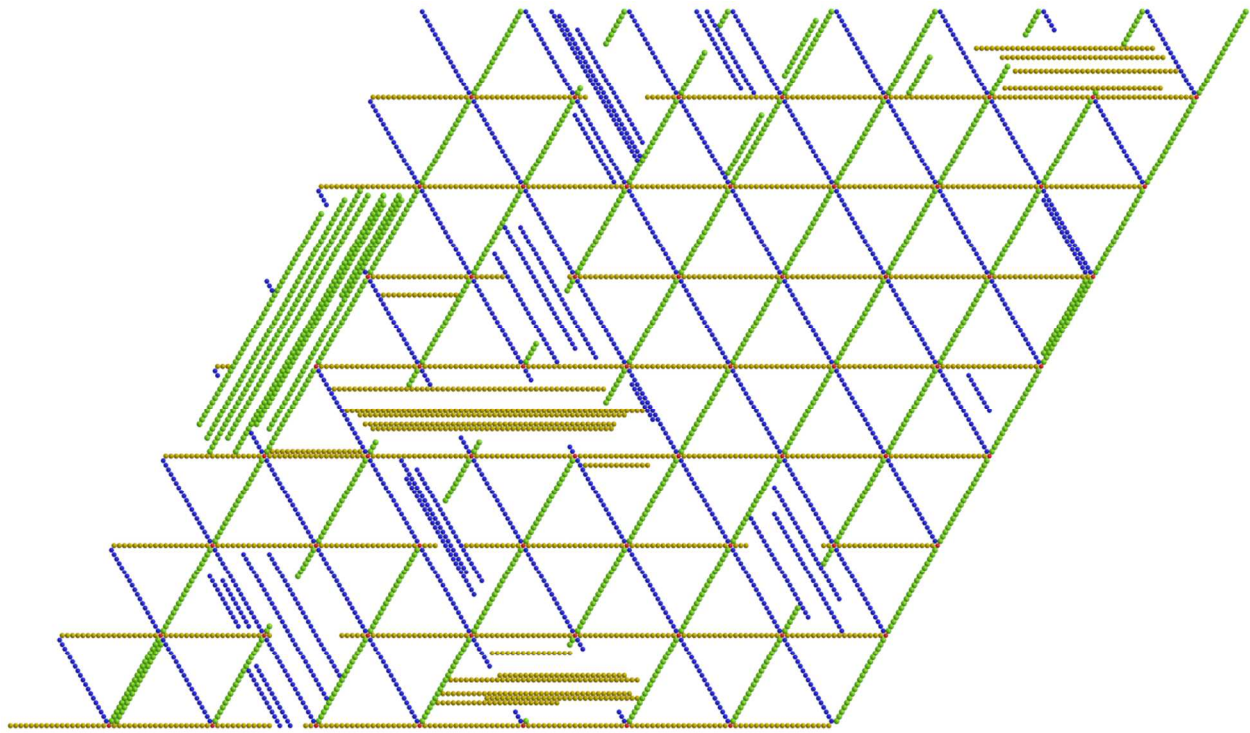


Fig. S5. Snapshot at $\theta = 0.19$, corresponding to inset 3 in Fig. 7 of the manuscript.

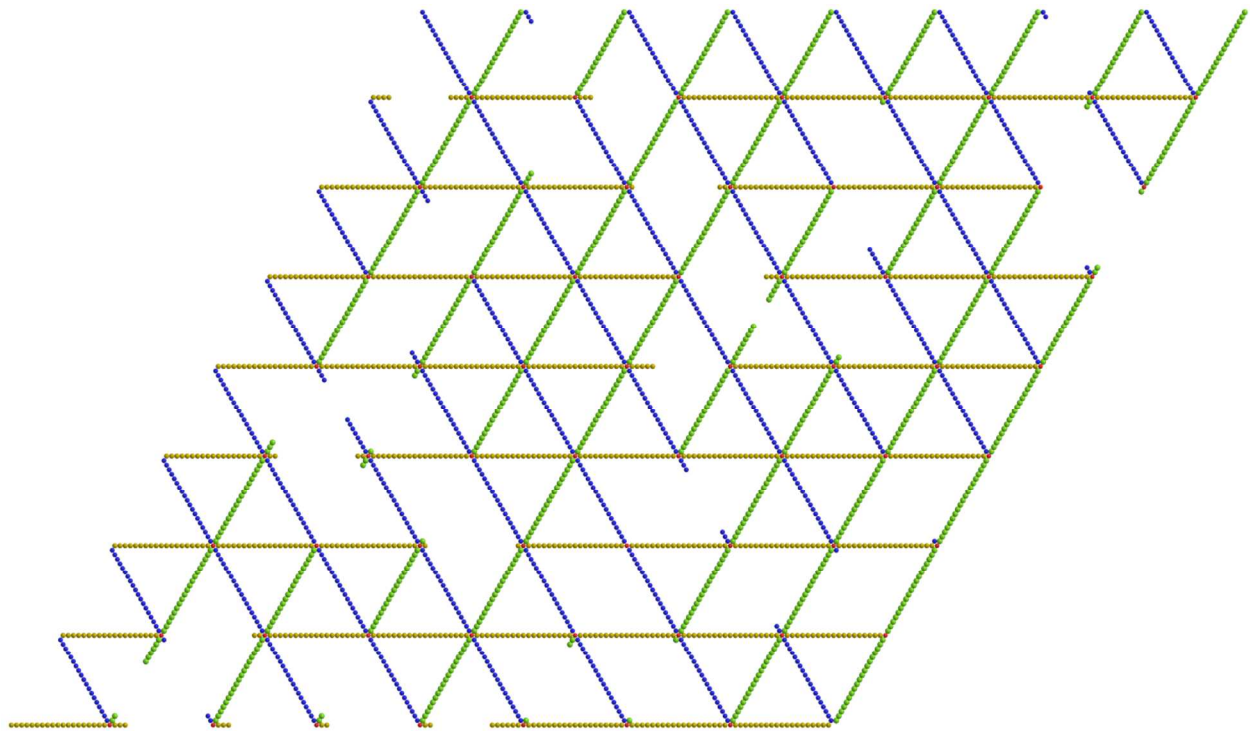


Fig. S6. Snapshot at $\theta = 0.12$, corresponding to inset 4 in Fig. 7 of the manuscript.

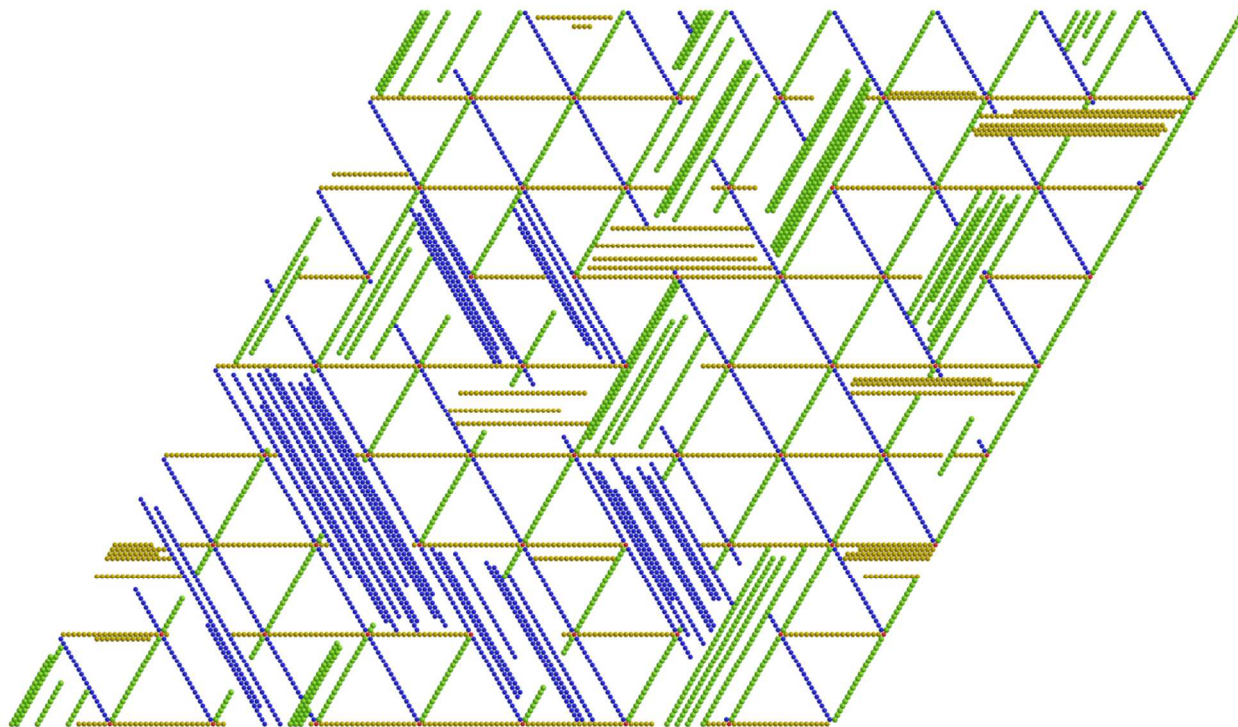


Fig. S7. Snapshot at $\theta = 0.24$, corresponding to inset 5 in Fig. 7 of the manuscript.