Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information:

The force field for graphyne

We characterize carbon atoms in the graphyne nanosheet as two types, labeled CA and CX. The atomic type CA is the same as the definition of carbon atoms in benzene. The second atom type CX is for carbon atoms in the acetylene linker. The force fields for CX atoms were taken from acetylene carbons.

The following force fields (in the OPLSAA format) were used together with the OPLSAA file ffbond.itp in MD simulations shown in the main text.

[atomtypes]

CA 12.01100 0.000 A 3.55000E-01 2.9288 E-01

CX 12.01100 0.000 A 3.55000E-01 3.1798E-01

[angletypes]

CA CX CX 1 180.00 524.67

[dihedraltypes]

CX CA CA CA 1 180.00 16.3600 2

CX CA CA CX 1 180.00 20.032 2

Initial configurations

Figures 1a-d show the initial configurations of the representative CaM/GYNS systems of MD simulation.

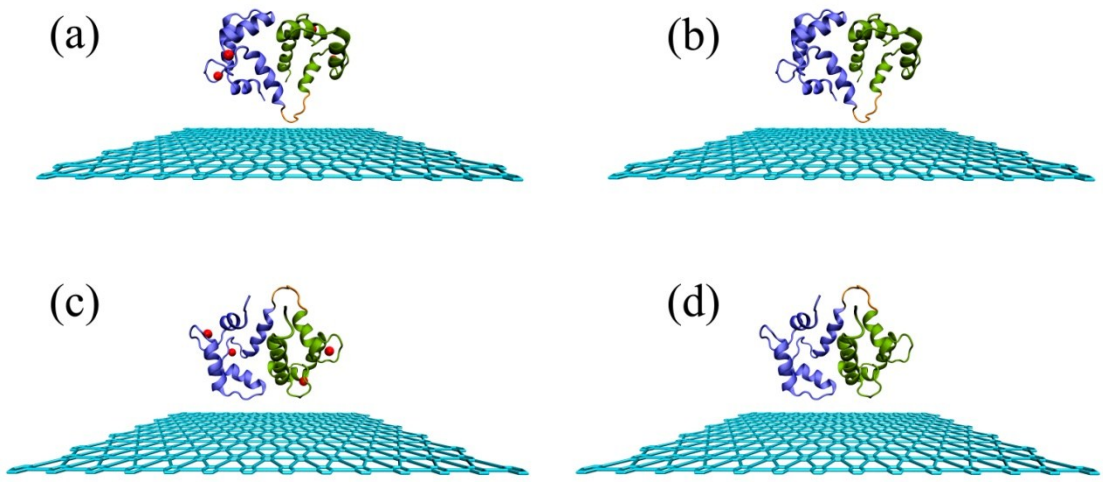

Figure 1.Initial structures of CaM/GYNS in Holo- and Apo- states and in both proximal and distal configurations: proximal Holo-CaM (a), proximal Apo-CaM (b), distal Holo-CaM (c), and distal Apo-CaM (d). The N-domain, C-domain and inter-domain linker of CaM are colored in green, blue and orange, respectively, with the GYNS in cyan and Ca^{2+} in red.

Figures 2a-b show the initial configurations of the representative CaM/GYQDs systems of MD simulation.

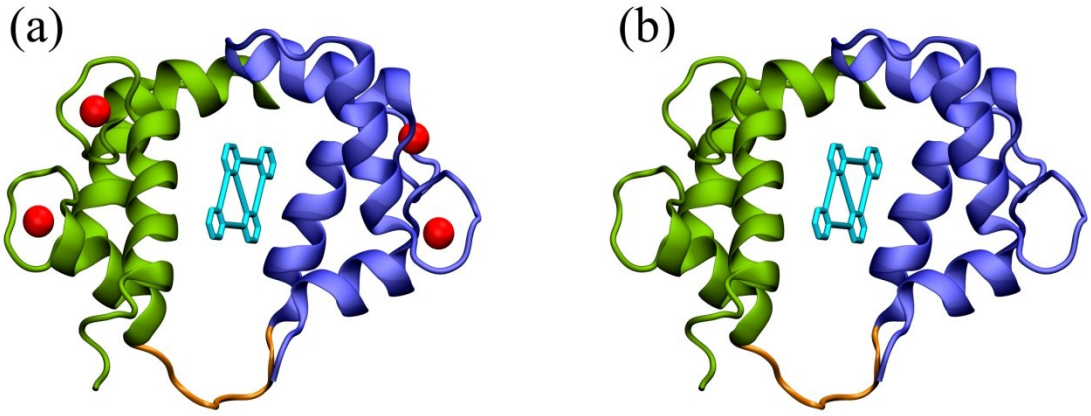

Figure 2. Initial structures of CaM/GYQDs in both Holo- (a) and Apo- (b) states.