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

Programed Dynamical Ordering in the Self-Organization Processes of a Nanocube: A Molecular Dynamics Study

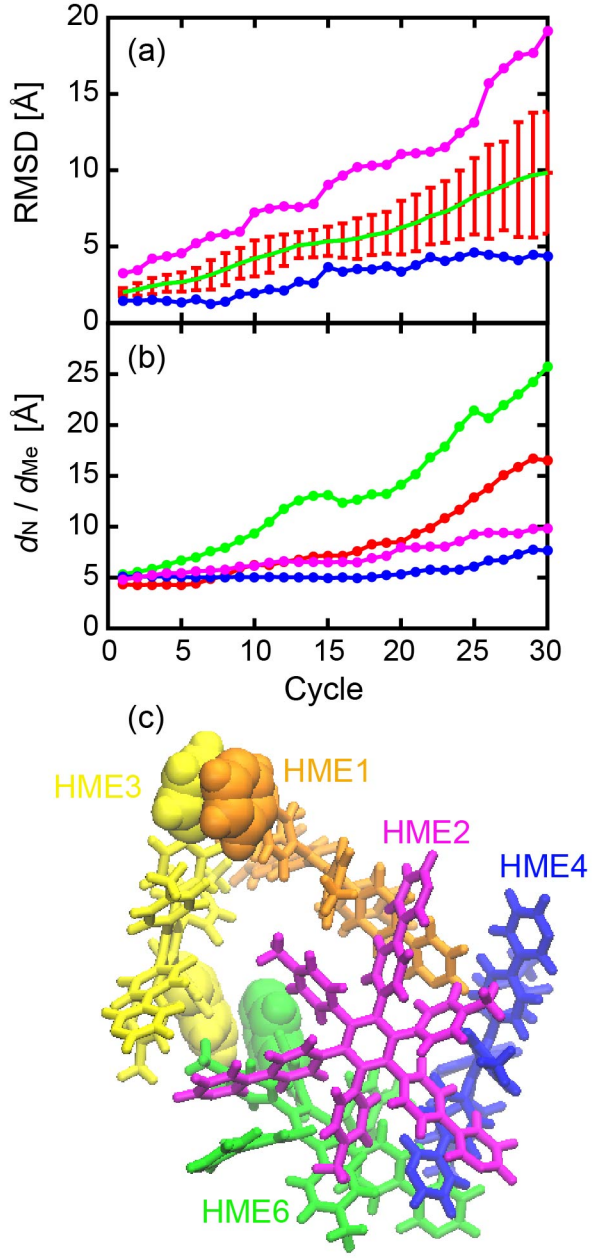
Ryuhei Harada[1]*†, Takako Mashiko[2], Masanori Tachikawa[2], Shuichi Hiraoka[3], Yasuteru Shigeta[1]*†

[1]*Center for Computational Sciences, University of Tsukuba, 1-1-1 Tennodai, Ibaraki 305-8577, Japan*

[2]*Quantum Chemistry Division, Graduate School of Science, Yokohama City University, 22-2 Seto, Kanazawa-ku, Yokoyama City, Kanagawa 236-0027, Japan*

[3]*Department of Basic Science, Graduate School of Arts and Sciences, The University of Tokyo, 3-8-1 Komaba, Meguro-ku, Tokyo 153-8902, Japan.*

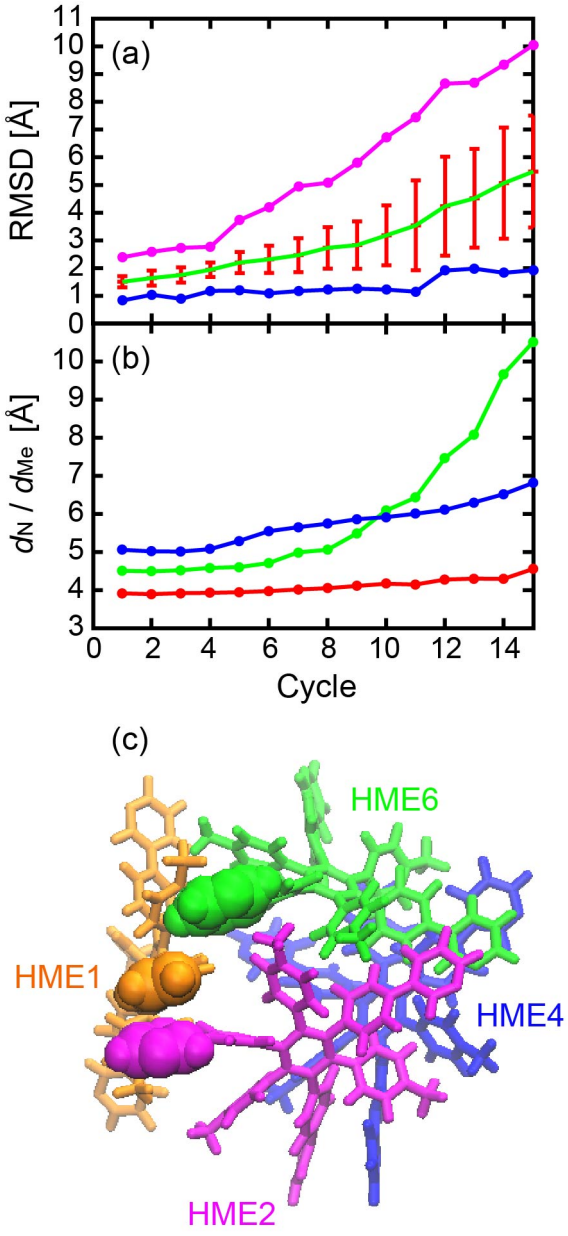
Figure S1



(a) Profiles of RMSD measured from $\mathbf{1}_5$ for the 30 cycles. (green) RMSD values averaged over all the snapshots sampled by SDS at every cycle and (red) its standard deviations. (blue) minimum and (magenta) maximum RMSD values at every cycle. (b) (blue, magenta) Profiles of averaged d_N of **HME1-HME2-HME4** and **HME2-HME4-HME6**, characterizing the triple π-stacking. (green, red) Profiles of d_{Me} of **HME1** and **HME3** and that of **HME3** and **HME6**, characterizing the CH-π interactions. (c) Initial structure of $\mathbf{1}_5$. **HME1**, **HME2, HME3**, **HME4,** and **HME6** are colored with orange, magenta, yellow, blue, and green, respectively. Some of Py groups are drawn by a VDW representation,

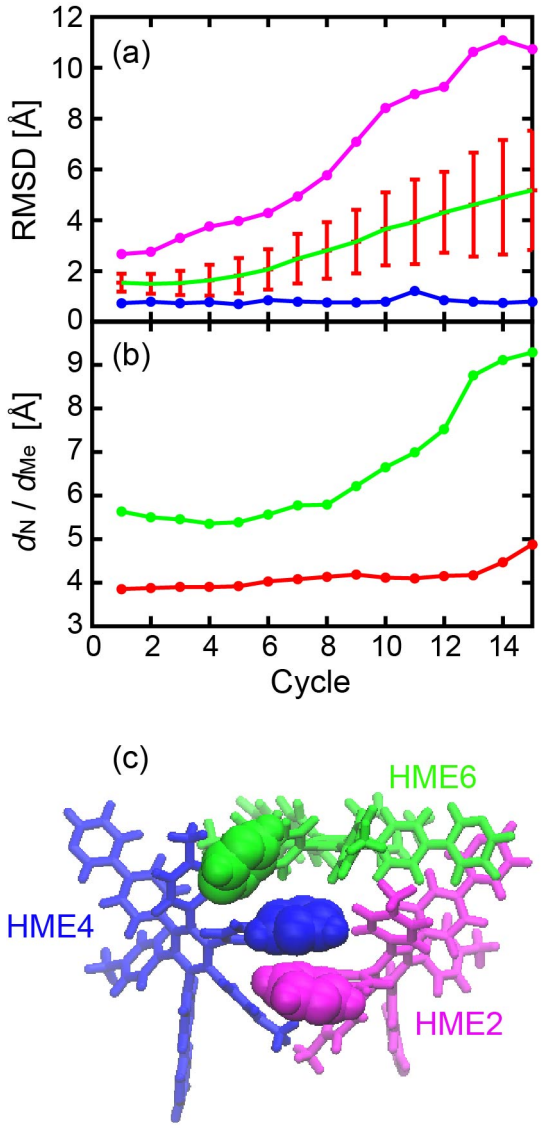
corresponding to the π-π stacking between **HME1**-**HME3** and that between **HME3** and **HME6**, they were collapsed in the second dissociation process from $\mathbf{1}_5$ to $\mathbf{1}_4$, leading to the dissociation of **HME3**.

Figure S2



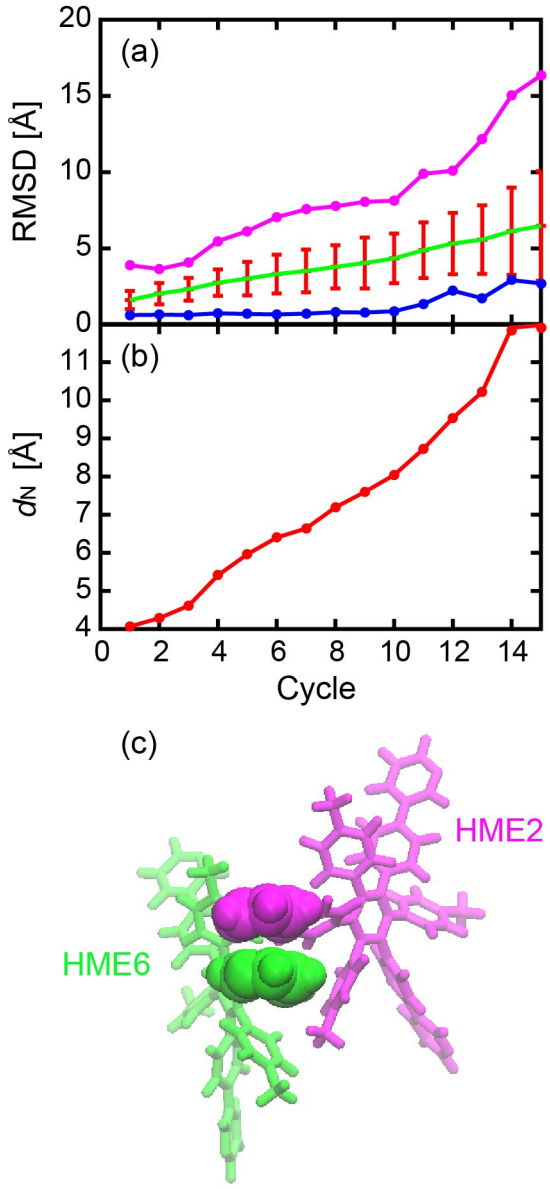
(a) Profiles of RMSD measured from $\mathbf{1}_4$ for the 15 cycles. (green) RMSD values averaged over all the snapshots sampled by SDS at every cycle and (red) its standard deviations. (blue) minimum and (magenta) maximum RMSD values at every cycle. (b) (red) Profile of d_{Me} between **HME2** and **HME4** characterizing the π-π stacking. (green, blue) Profiles of averaged d_N characterizing the triple π-stacking among **HME1-HME2-HME6** and among **HME2-HME4-HME6**, respectively. (c) Initial structure of $\mathbf{1}_4$. **HME1**, **HME2**, **HME4**, and **HME6** are colored with orange, magenta, blue, and green, respectively. Some Py groups are drawn by a VDW representation, corresponding to the triple π-stacking among them, which was collapsed in the third dissociation process from $\mathbf{1}_4$ to $\mathbf{1}_3$, leading to the dissociation of **HME1**.

Figure S3



(a) Profiles of RMSD measured from $\mathbf{1}_3$ for the 15 cycles. (green) RMSD values averaged over all the snapshots sampled by SDS at every cycle and (red) its standard deviations. (blue) minimum and (magenta) maximum RMSD values at every cycle. (b) (red) Profile of d_{Me} characterizing CH-π interaction between **HME2** and **HME6** and (green) that of averaged d_N characterizing triple π-stacking among **HME2**, **HME4**, and **HME6**. (c) Initial structure of $\mathbf{1}_3$. Each monomer is colored with (magenta) **HME2**, (blue) **HME4**, and (green) **HME6**, respectively. Some Py groups are drawn with a VDW representation, characterizing the triple π-stacking among them, which was also collapsed in the forth dissociation process, leading to the dissociation of **HME4**.

Figure S4



(a) Profiles of RMSD measured from $\mathbf{1}_2$ for the 15 cycles. (green) RMSD values averaged over all the snapshots sampled by SDS at every cycle and (red) its standard deviations. (blue) minimum and (magenta) maximum RMSD values at every cycle. (b) Profile of nitrogen-nitrogen distance between Py of **HME2** and **HME6** characterizing the π-π stacking. (c) Initial structure of $\mathbf{1}_2$, where **HME2** and **HME6** are colored in magenta and green, respectively. Two Py groups are drawn with a VDW representation to highlight the π-π stacking.

Movies of each dissociation process

(a) 6mer.mov: Dissociation process from $\mathbf{1}_6$ to $\mathbf{1}_5$+**1**.

(b) 5mer.mov: Dissociation process from $\mathbf{1}_5$ to $\mathbf{1}_4$+**1**.

(c) 4mer.mov: Dissociation process from $\mathbf{1}_4$ to $\mathbf{1}_3$+**1**.

(d) 3mer.mov: Dissociation process from $\mathbf{1}_3$ to $\mathbf{1}_2$+**1**.

(e) 2mer.mov: Dissociation process from $\mathbf{1}_2$ to $\mathbf{1}_1$+**1**.