Molecular and Mesoscale Mechanism for Hierarchical Self-Assembly of Dipeptide and Porphyrin Light-Harvesting System

Kai Liu¹,², Yu Kang³*, Guanghui Ma¹, Helmuth Möhwald⁴, Xuehai Yan¹,²,*

1 State Key Laboratory of Biochemical Engineering, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China
2 Center for Mesoscience, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China
3 College of Pharmaceutical Sciences, Zhejiang University, Hangzhou, Zhejiang 310058, China
4 Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1, Potsdam/Golm 14476, Germany

Corresponding Author
*Email: yanxh@ipe.ac.cn; yukang@zju.edu.cn
Homepage: http://www.yan-assembly.org/
Figure S1. Models for molecular clusters and electrostatic surface potential. Clusters of (a) two H$_2$TPPS$^{2-}$ molecules, (b) one H$_2$TPPS$^{2-}$ molecule and one KK$^{3+}$ molecule and (c) one H$_2$TPPS$^{2-}$ molecule and one FF$^+$ molecule.
Figure S2. Structure of assembled (a) $\text{H}_2\text{TPPS}^{2-}$ and KK$^{3+}$ (b) $\text{H}_2\text{TPPS}^{2-}$ and FF$^+$ from MD Simulation. Water molecules are omitted. The CPK model has been used for dipeptides, and the line model has been used for $\text{H}_2\text{TPPS}^{2-}$. 
Figure S3. Distribution of species (a) along the x axis in the H$_2$TPPS$^{2-}$-KK$^{3+}$ system, (b) along the y axis in the H$_2$TPPS$^{2-}$-KK$^{3+}$ system, (c) along the z axis in the H$_2$TPPS$^{2-}$-KK$^{3+}$ system, (d) along the x axis in the H$_2$TPPS$^{2-}$-FF$^+$ system, (e) along the y axis in the H$_2$TPPS$^{2-}$-FF$^+$ system, and (f) along the z axis in the H$_2$TPPS$^{2-}$-FF$^+$ system. The axes are shown in Figure S2.
**Figure S4.** Mesoscopic structures of (a) H$_2$TPPS$^{2-}$-KK$^{3+}$ assembly and (b) H$_2$TPPS$^{2-}$-FF$^+$ assembly in aqueous solution.
Figure S5. Molecular distribution of \( \text{H}_2\text{TPPS}^2^- \), KK\(^{3+} \) and water along the axis (a)x, (b)y, (c)z in the \( \text{H}_2\text{TPPS}^2^-\)-KK\(^{3+} \) assembly in aqueous solution, and molecular distribution of \( \text{H}_2\text{TPPS}^2^- \), FF\(^+ \) and water along the axis (d)x, (e)y, (f)z in the \( \text{H}_2\text{TPPS}^2^-\)-FF\(^+ \) assembly in aqueous solution. The axes are shown in Figure S4.
Figure S6. Mesoscopic structures of H$_2$TPPS$^{2-}$ assembly in aqueous solution with a proportion of (a) H$_2$TPPS$^{2-}$: water=50:1 and (b) H$_2$TPPS$^{2-}$: water = 10:1.