

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

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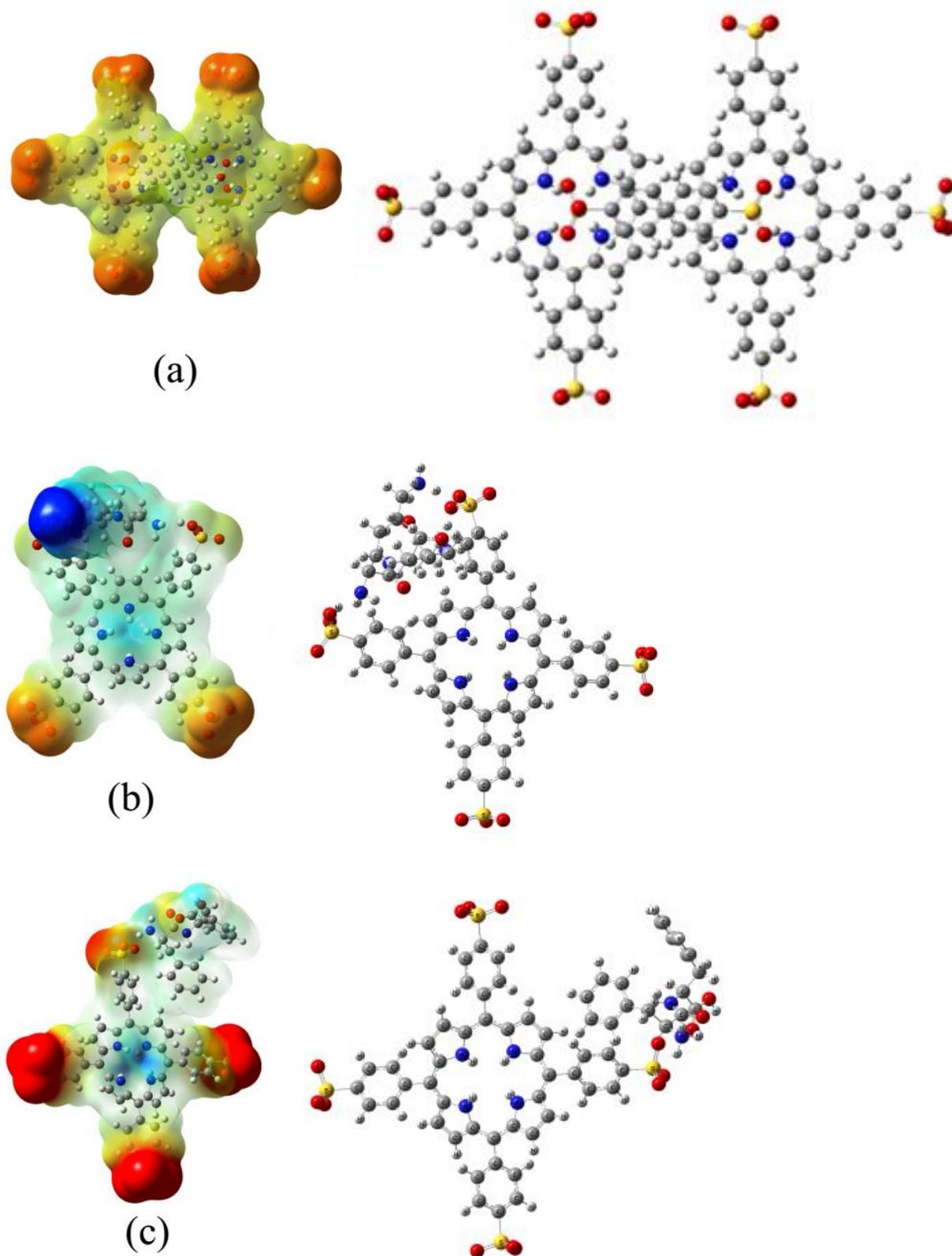


Figure S1. Models for molecular clusters and electrostatic surface potential. Clusters of (a) two $\text{H}_2\text{TPPS}^{2-}$ molecules, (b) one $\text{H}_2\text{TPPS}^{2-}$ molecule and one KK^{3+} molecule and (c) one $\text{H}_2\text{TPPS}^{2-}$ molecule and one FF^+ molecule.

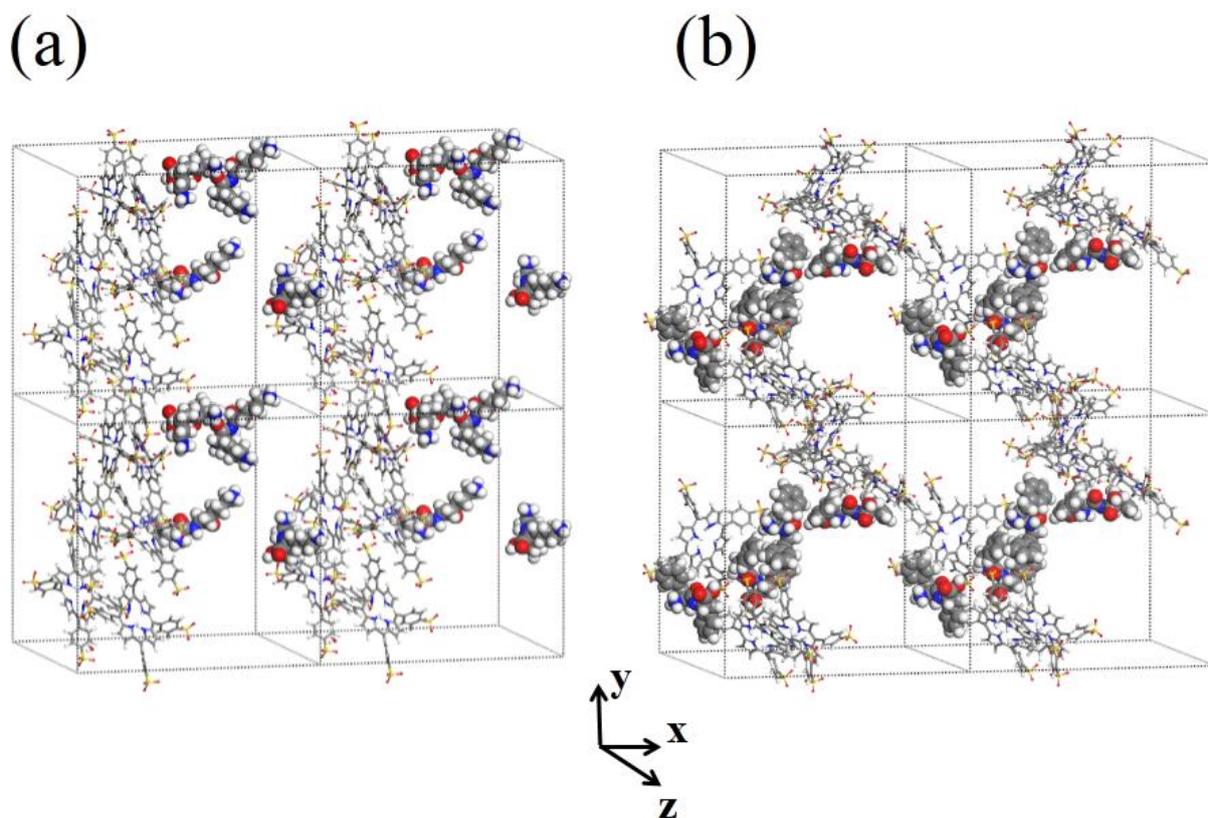


Figure S2. Structure of assembled (a) H₂TPPS²⁻ and KK³⁺ (b) H₂TPPS²⁻ and FF⁺ from MD Simulation. Water molecules are omitted. The CPK model has been used for dipeptides, and the line model has been used for H₂TPPS²⁻.

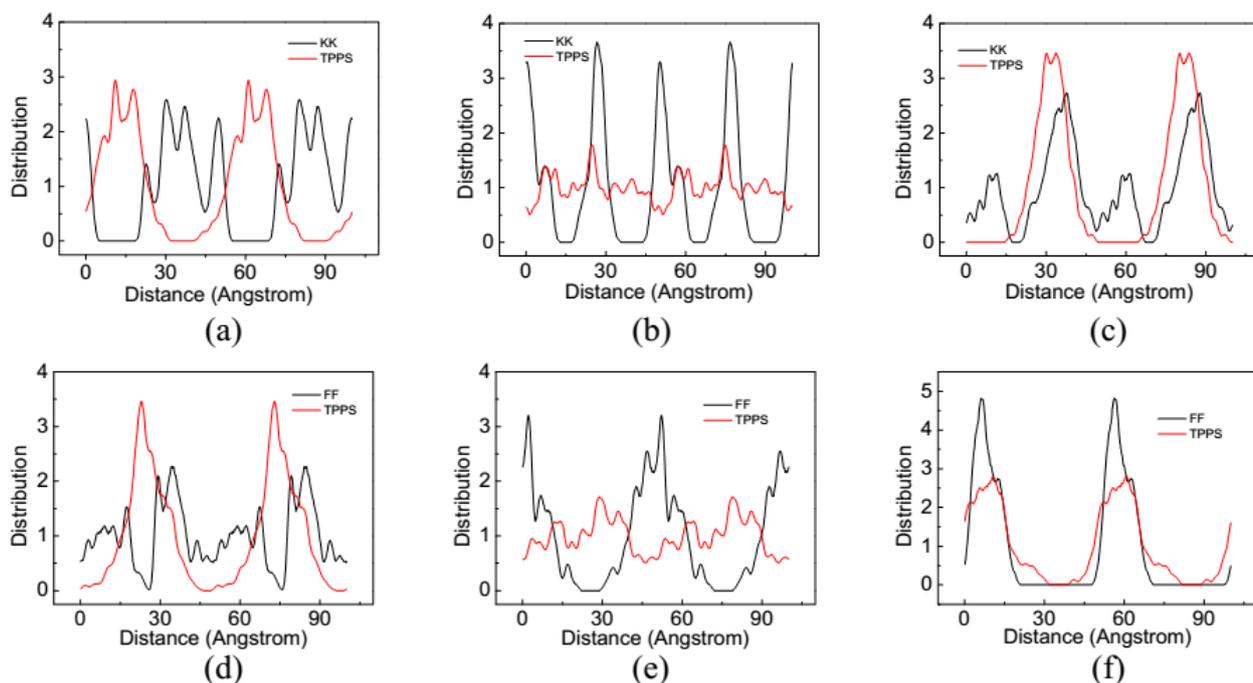


Figure S3. Distribution of species (a) along the x axis in the $H_2TPPS^{2-}-KK^{3+}$ system, (b) along the y axis in the $H_2TPPS^{2-}-KK^{3+}$ system, (c) along the z axis in the $H_2TPPS^{2-}-KK^{3+}$ system, (d) along the x axis in the $H_2TPPS^{2-}-FF^+$ system, (e) along the y axis in the $H_2TPPS^{2-}-FF^+$ system, and (f) along the z axis in the $H_2TPPS^{2-}-FF^+$ system. The axes are shown in Figure S2.

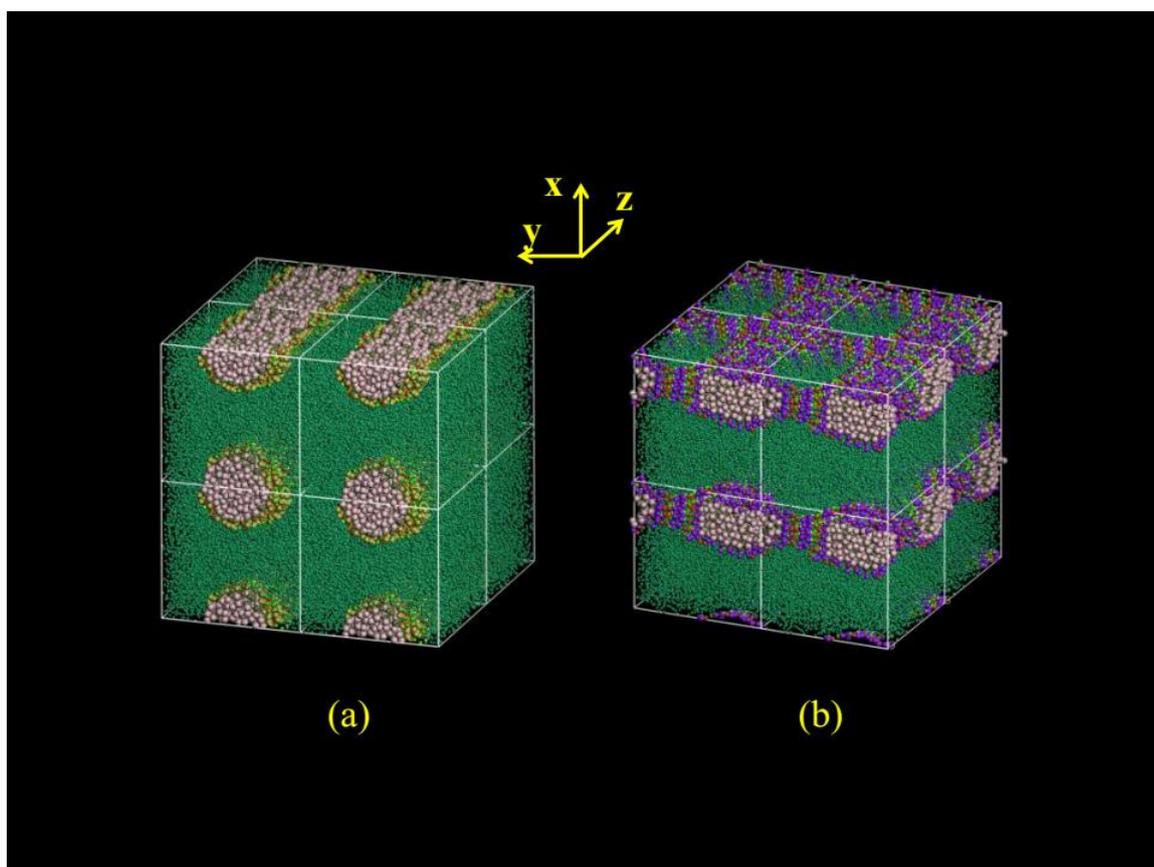


Figure S4. Mesoscopic structures of (a) $\text{H}_2\text{TPPS}^{2-}\text{-KK}^{3+}$ assembly and (b) $\text{H}_2\text{TPPS}^{2-}\text{-FF}^+$ assembly in aqueous solution.

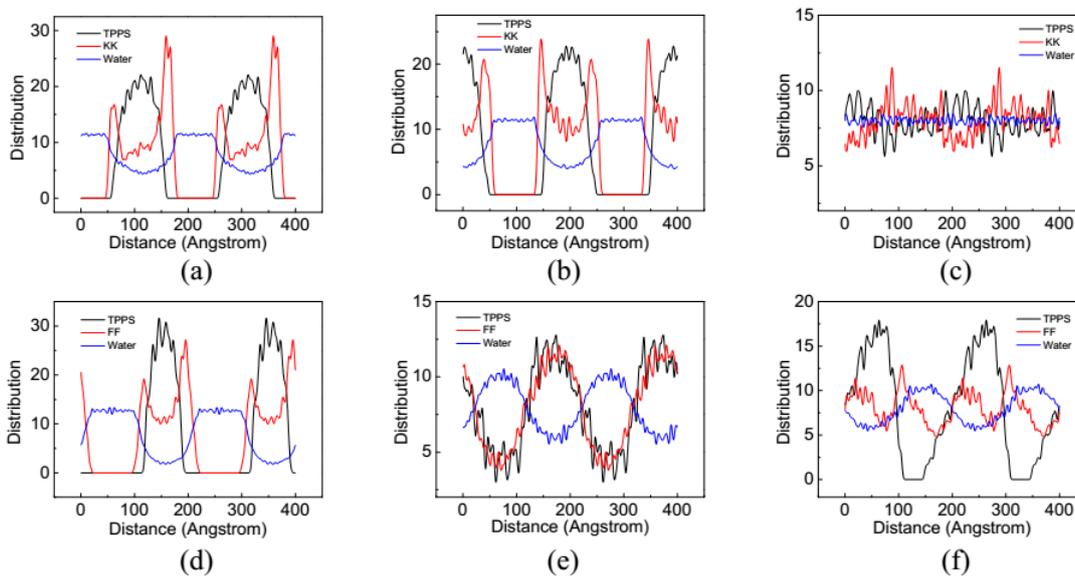


Figure S5. Molecular distribution of $\text{H}_2\text{TPPS}^{2-}$, KK^{3+} and water along the axis (a)x, (b)y, (c)z in the $\text{H}_2\text{TPPS}^{2-}$ - KK^{3+} assembly in aqueous solution, and molecular distribution of $\text{H}_2\text{TPPS}^{2-}$, FF^+ and water along the axis (d)x, (e)y, (f)z in the $\text{H}_2\text{TPPS}^{2-}$ - FF^+ assembly in aqueous solution. The axes are shown in Figure S4.

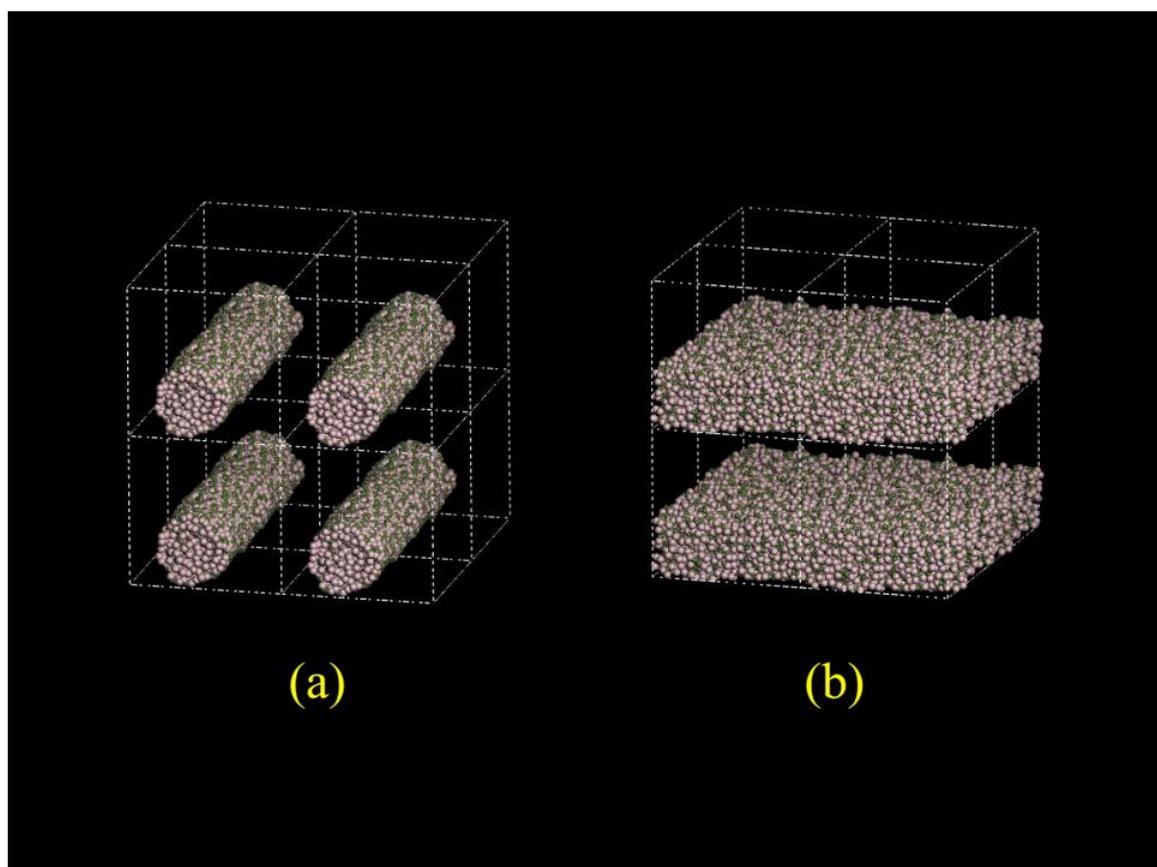


Figure S6. Mesoscopic structures of $\text{H}_2\text{TPPS}^{2-}$ assembly in aqueous solution with a proportion of (a) $\text{H}_2\text{TPPS}^{2-}$: water=50:1 and (b) $\text{H}_2\text{TPPS}^{2-}$: water = 10:1.