## **Electronic Supporting Information**

## Ultrafast Electron Transfer Across a Nanocapsular Wall: Coumarins as Donors, Viologen as Acceptor and Octa Acid Capsule as the Mediator

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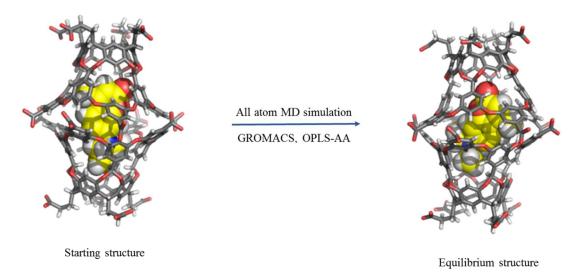


Figure S1. Starting and equilibrium structures of C1@OA<sub>2</sub> complexes.

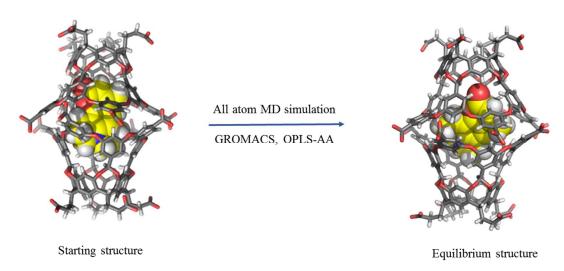


Figure S2. Starting and equilibrium structures of C480@OA<sub>2</sub> complexes.

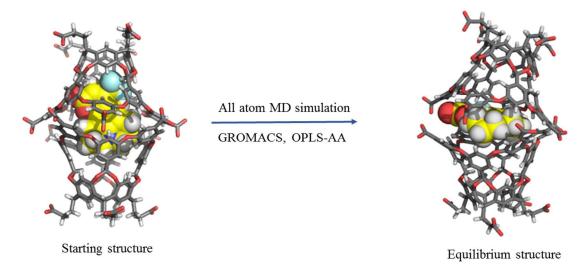


Figure S3. Starting and equilibrium structures of C153@OA<sub>2</sub> complexes.

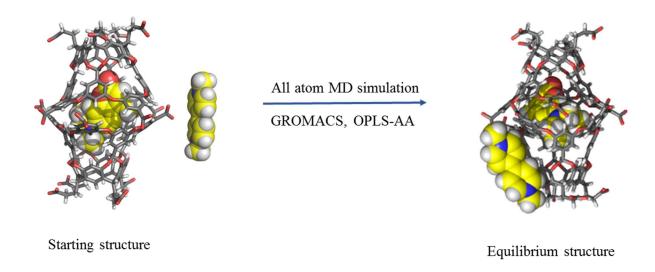
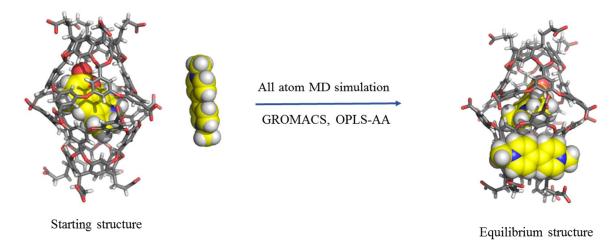
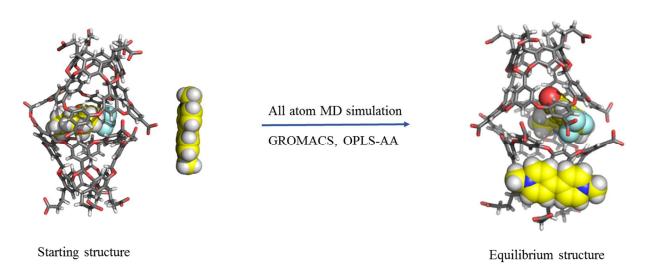


Figure S4. Starting and equilibrium structures of  $C1@OA_2-MV^{2+}$  complexes.



**Figure S5**. Starting and equilibrium structures of C480@OA<sub>2</sub>-MV<sup>2+</sup> complexes.



**Figure S6**. Starting and equilibrium structures of C153@OA<sub>2</sub>-MV<sup>2+</sup> complexes.