## **Description of Additional Supplementary Files**

File Name: Supplementary Movie 1

Description: Atomistic molecular dynamics simulation of cage 2 at room temperature in

explicit water. The movie is available for downloading at https://www.dropbox.com/s/ogmnrp27y71buh3/2.mov.

File Name: Supplementary Movie 1

Description: Atomistic molecular dynamics simulation of cage 4 at room temperature in

explicit water. The movie is available for downloading at https://www.dropbox.com/s/sa41typlu0j6all/4.mov.