

# **Supplemental Materials:**

## **Molecular Origin of the Prepeak in the**

## **Structure Factor of Alcohols**

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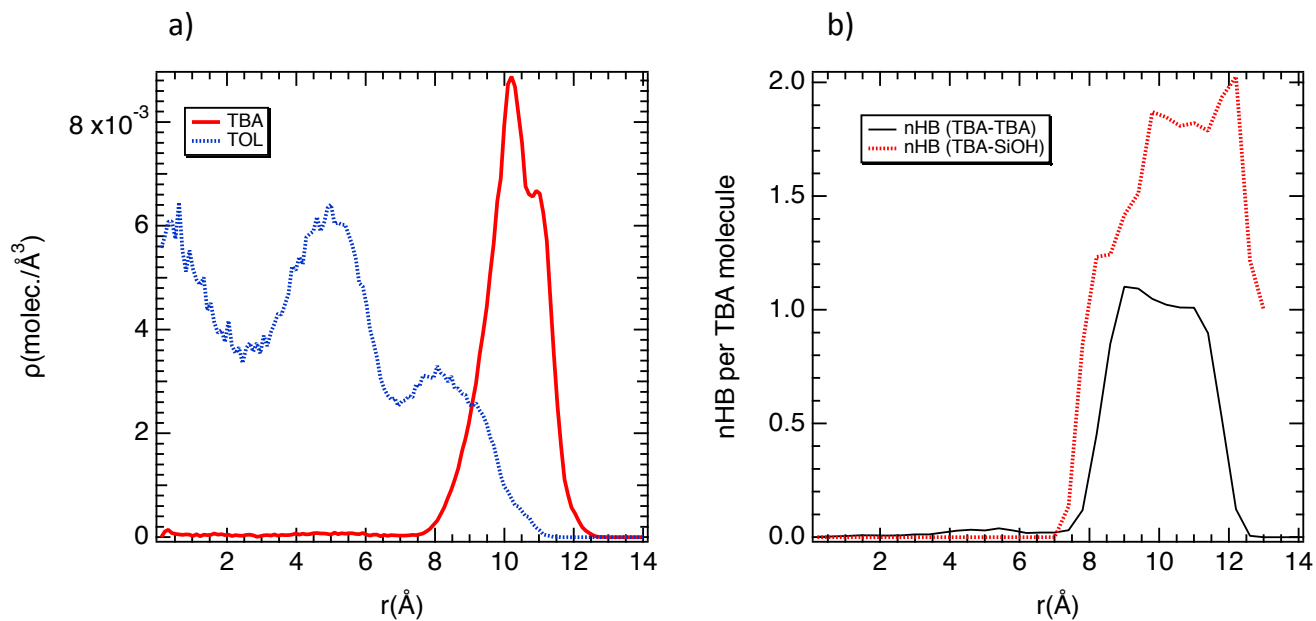


Figure S1: a) Profile of the density of centre of mass of TBA and TOL confined in the SiOH-R12 along the radial direction. b) Profile of the hydrogen bonds number between TBA molecules and between TBA and the silanol groups (SiOH) along the radial direction of the SiOH-R12 porous material.

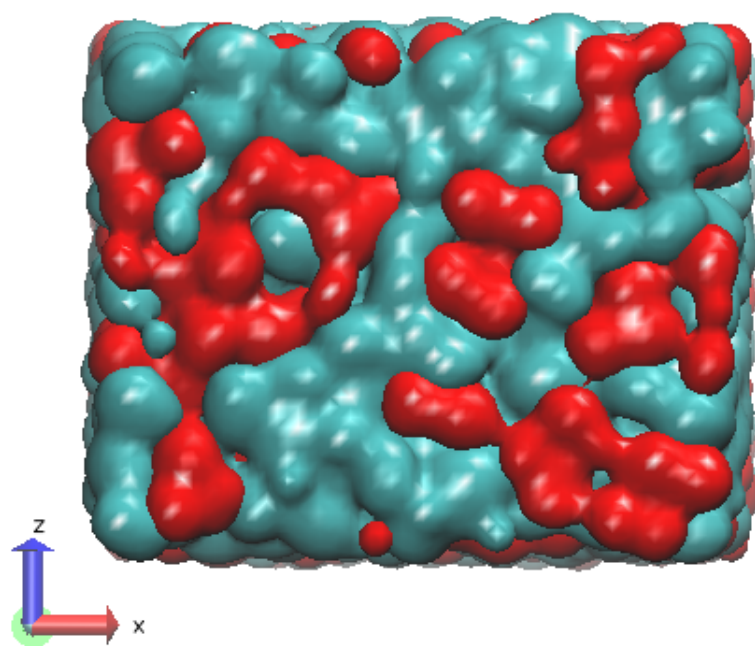


Figure S2: Connolly's surface representation of TBA/TOL binary mixture such that TOL and TBA molecules are represented in cyan and red colors, respectively.

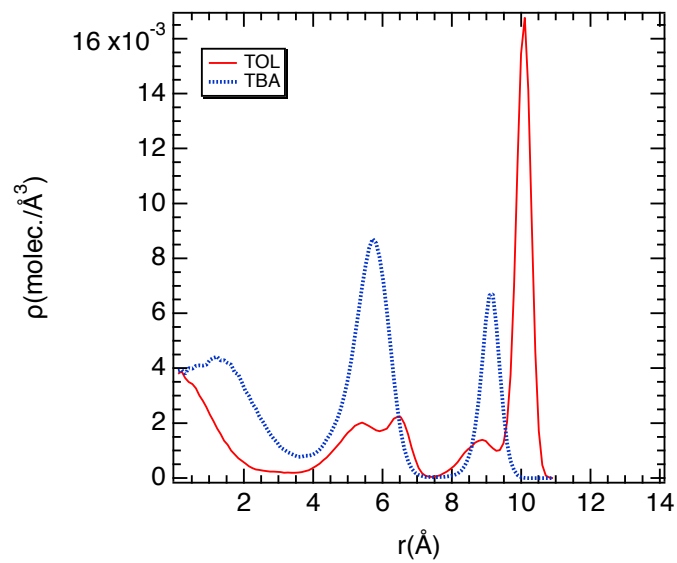


Figure S3: Profile of the density of centre of mass of TBA and TOL confined in the CNT along the radial direction.

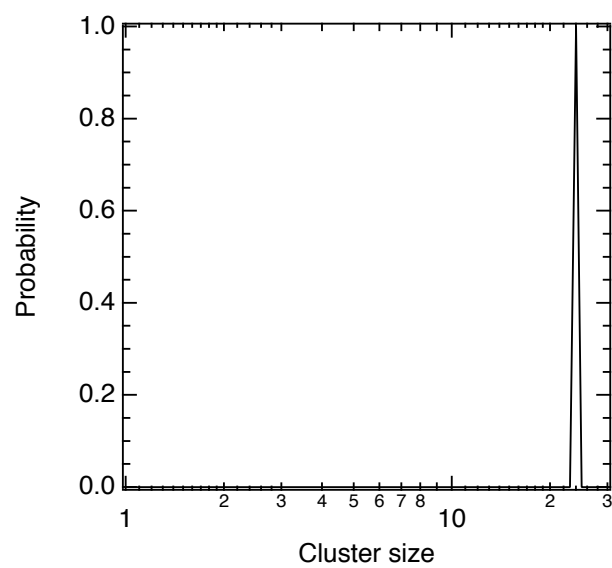


Figure S4: Cluster size distribution of TBA molecules for the TBA/TOL binary mixture confined in SiOH-R6.

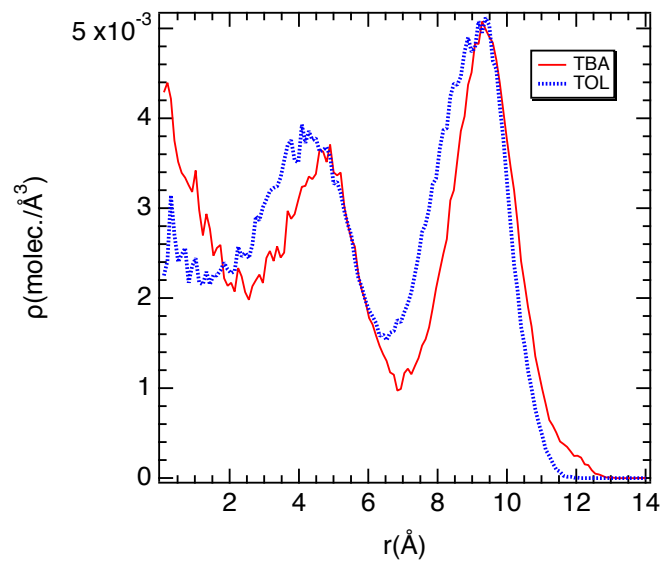


Figure S5: Profile of the density of centre of mass of TBA and TOL confined in the weakly hydrated (WH) silica porous material of radius of 12 Å along the radial direction.