Physical Chemistry Chemical Physics
Supporting Information

Local structure and dynamics of benzene confined in IRMOF-1 nanocavity as studied by molecular dynamics simulation

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Temperature dependence of pair correlation function of benzene is shown in Fig. S1 for benzene loading of 13 and 63 molecules per unit cell. The features of the profiles in each loading level are similar to each of them for loading of 20 and 56 molecules per unit cell.
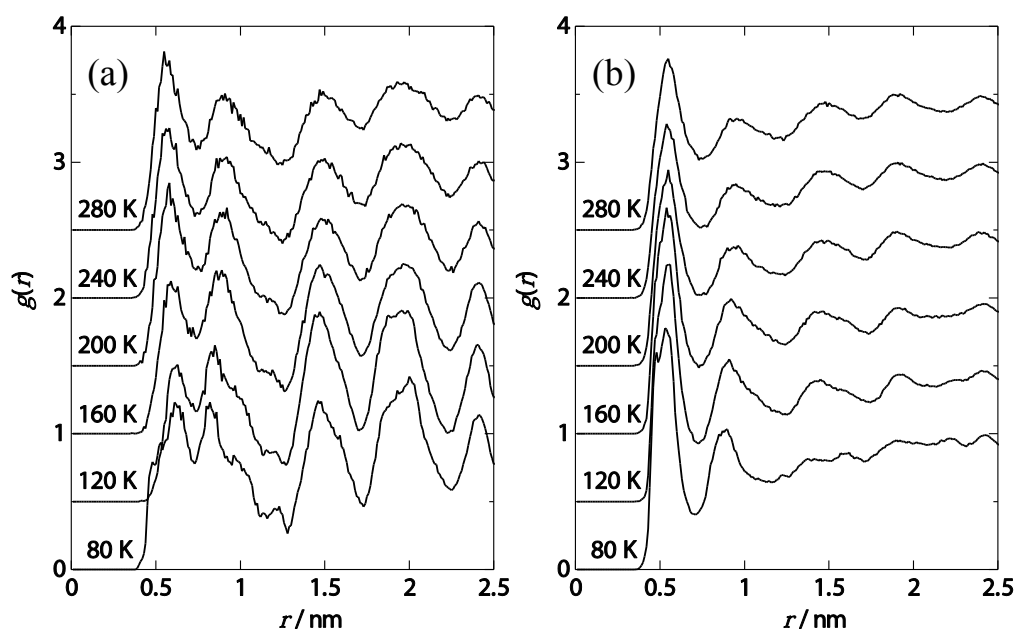

Fig. S1 Temperature dependence of pair correlation function, g(r), for benzene loading of 13 molecules (a) and 63 molecules (b) per unit cell.

The maximum occupations of benzene in each of the large and small cavities are presented in Fig. S2 for benzene loading of 13 and 63 molecules per unit cell. The tendency of the change in the occupation is similar to those for loading of 20 and 56 molecules per unit cell. The inhomogeneous distribution of benzene in the unit cell is found in the high loading region.
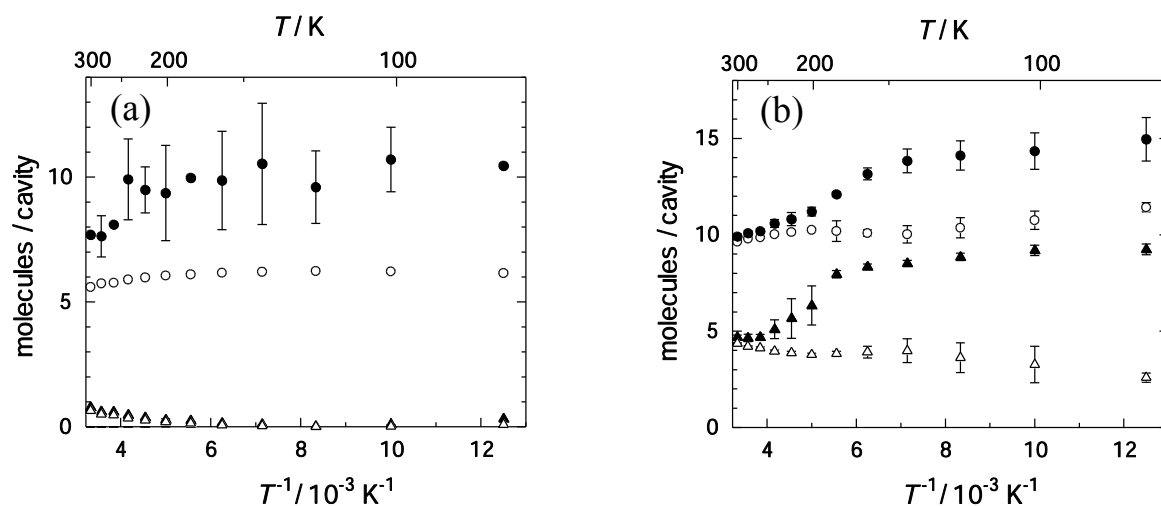
Fig. S2 Maximum occupation of benzene in each of the large and small cavities for benzene loading of 13 molecules (a) and 63 molecules (b) per unit cell.

The iso-density surface map and the diffusion pathway of a benzene molecule are depicted in Fig. S3 and S4 for benzene loading of 13 and 63 molecules per unit cell.
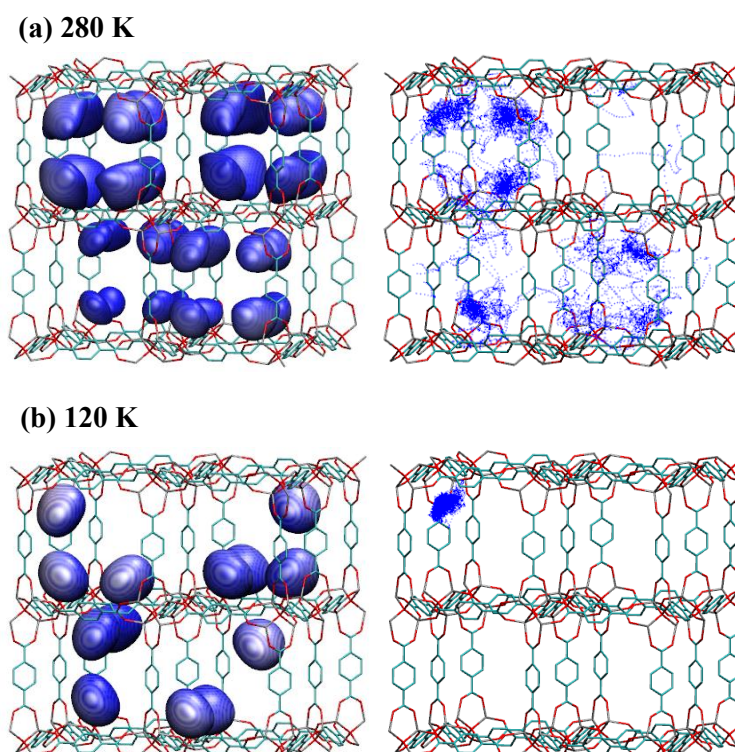
(a) 280 K

(b) 120 K

Fig. S3 Iso-density surface map and the diffusion pathway of a benzene molecule for the benzene loading of 13 molecules (20% saturation at room temperature) per unit cell.
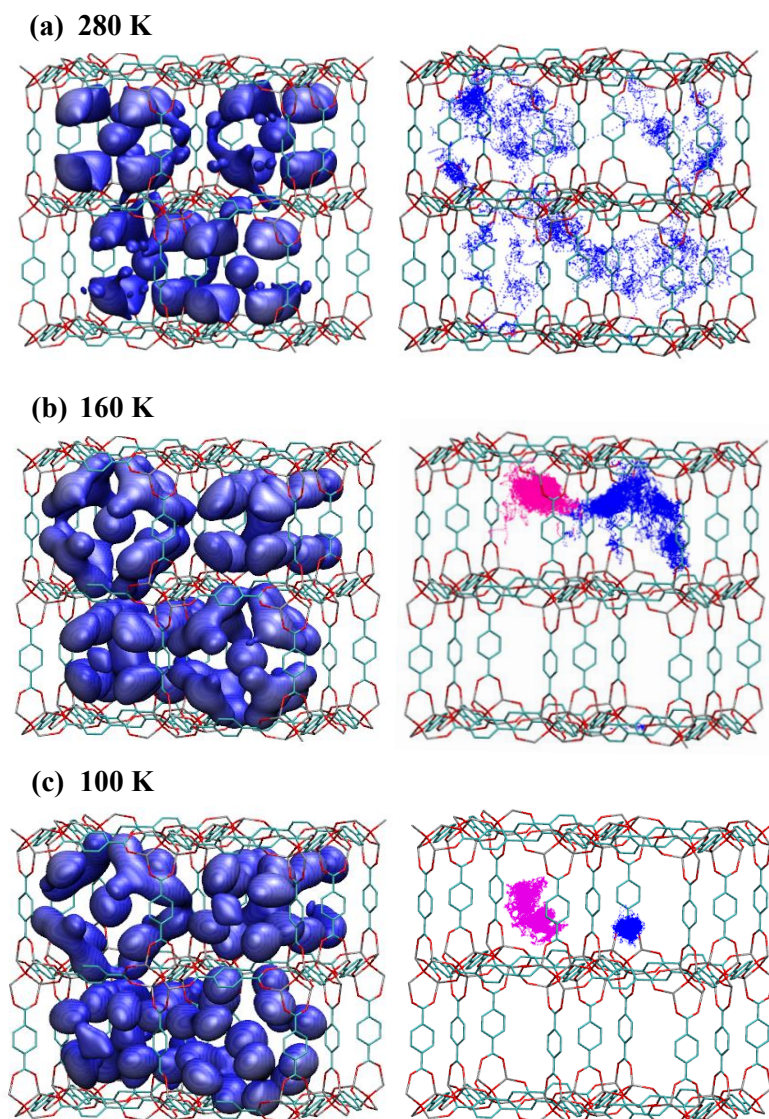
(a) 280 K

(b) 160 K

(c) 100 K

Fig. S4 Iso-density surface map and diffusion pathway of a benzene molecule for the benzene loading of 63 molecules (100% saturation at room temperature) per unit cell.

The supplementary simulations were carried out with the MD time of 10 ns at 100 K and 200 K for the benzene loading of 56 molecules per unit cell. The other conditions were the same as other simulations in this work. The diffusion pathway of benzene is shown in Fig. S5. At 200 K, a trajectory of centre of mass for a benzene molecule is distributed over the whole unit cell, although the resident frequencies of benzene are different between the large and the small cavities. In contrast, at 100 K, a benzene molecule migrated in the large cavity, whereas the benzene molecules in the small cavity were localized at D sites. Thus, the benzene molecules could not undergo the inter-cavity diffusion even at the MD time of 10 ns. This result implies that the resident time of benzene in each cavity is longer than 10 ns at 100 K. This fact strongly supports our conclusion in the present work.
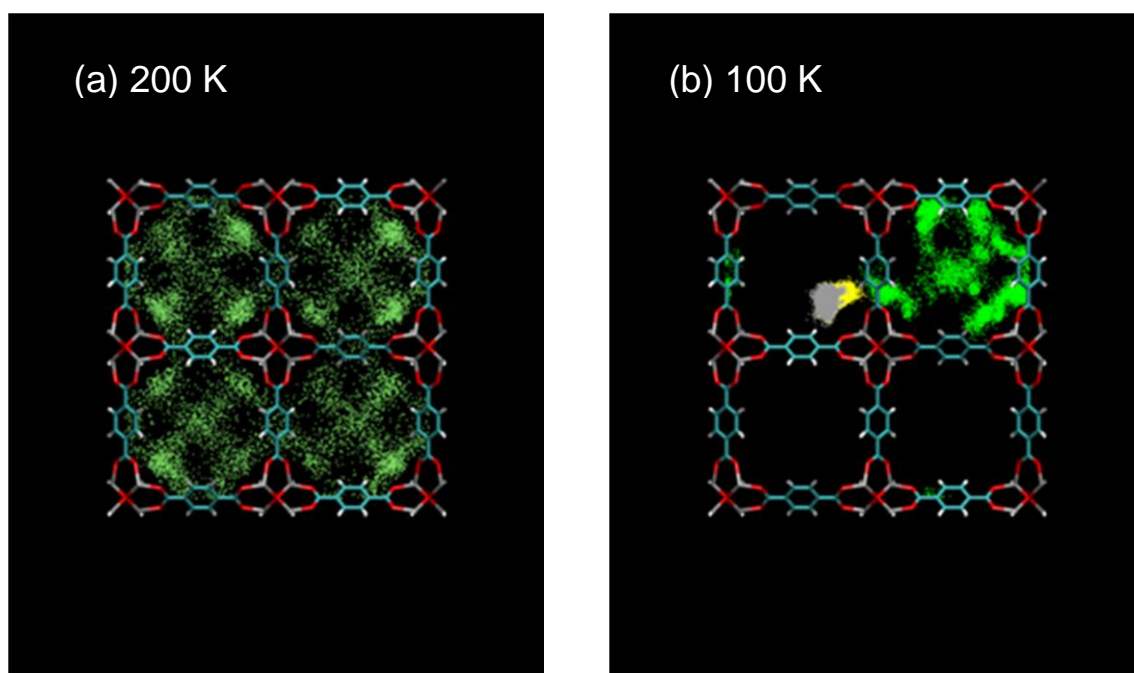
Fig. S5 Diffusion pathway of benzene simulated with the MD time of 10 ns for the benzene loading of 56 molecules per unit cell: 200 K (a) and 100 K (b). At 200 K, the trajectory of a benzene molecule is represented, whereas at 100 K two benzene molecules (gray and yellow dots) are localized at D sites and a benzene molecule (green dots) migrates in the large cavity.