Supporting Information

On the diffusion of ionic liquids in ILs@ZIF-8 composite materials: a density functional theory study

Longlong Liu,[a] Kun Jiang,[a] Qingjun Chen,[b] Lei Liu[a*]

[a] Center for Computational Chemistry, College of Chemistry and Chemical Engineering, Wuhan Textile University, Wuhan, 430200 P. R. China
[b] Key Laboratory of Rare Earths, Ganjiang Innovation Academy, Chinese Academy of Sciences, Ganzhou 341000, China

Corresponding author:

Lei Liu, liulei3039@gmail.com; liulei@wtu.edu

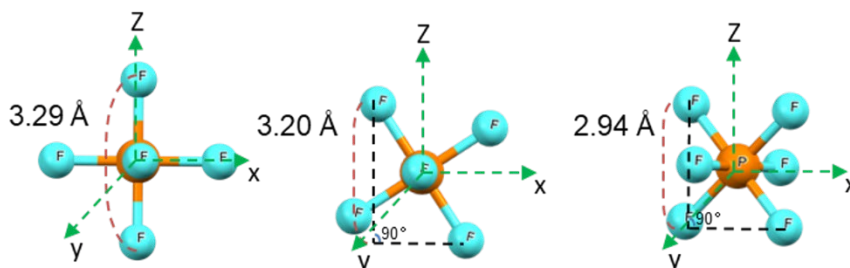**Figure S1** Three different ways and their diameters of the [PF6] pathing through the ZIF-8 pore.

Figure S2. Interaction energy components calculated using the GKS-EDA method at the B3LYP-D3(BJ)/6-311+G* level for the different $[PF_6]^-$ ways towards the ZIF-8 aperture.

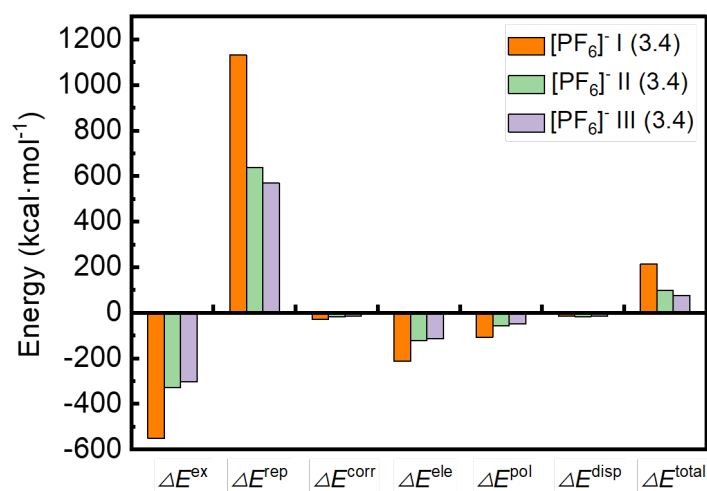**Figure S3.** The structures for the points with the highest interaction energies in the cases of $[PF_6]^-/[C_4mim]^+$ and ZIF-8(3.4), respectively, and the average distance refers to the closest distances between the fluorine atom on the $[PF_6]^-$, or the hydrogen atoms on the $[C_4mim]^+$ and the hydrogen atom on the aperture.

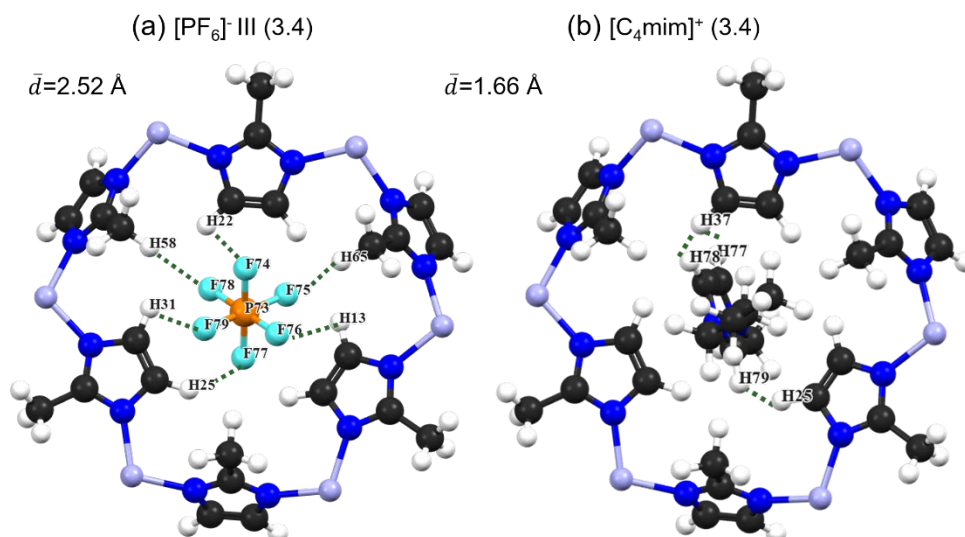(a) [PF$_6$]$^-$ III (3.4)   (b) [C$_4$mim]$^+$ (3.4)

$\bar{d}$=2.52 Å $\bar{d}$=1.66 Å

Table S1. NPA charge analysis of [PF$_6$]$^-$/[C$_4$mim]$^+$ and ZIF-8(3.4) at theoretical levels of B3LYP-D3(BJ)/6-311+G*.(values are in e)

System	q(anion)	q(cation)	$\triangle q$(ZIF-8)
[PF$_6$]$^-$ III (3.4)	-0.914	--	-0.086[a]
[C$_4$mim]$^+$ (3.4)	--	0.916	0.084[b]

*The initial charge of the ZIF-8 surface is zero.

q(anion) and q(cation) is the charge distribution of [PF$_6$]$^-$ and [C$_4$mim]$^+$ after the NPA charge calculation results, respectively.

[a]$\triangle$q(ZIF-8) is the sum of the charge distribution in the [PF$_6$]$^-$-ZIF-8(3.4) system.

[b]$\triangle$q(ZIF-8) is the sum of the charge distribution in the [C$_4$mim]$^+$-ZIF-8(3.4) system.