Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Molecular perspective on charge-tunable adsorption of volatile organic compounds on carbon nanotubes

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Table S1 Force field parameters describing the interactions between VOCs and the CNT.

Atom name	Atom type	σ(nm)	ε(kJ/mol)	Atom name	Atom type	σ(nm)	ε(kJ/mol)
CNT				**Ether**			
C	CA	0.355	0.293	$C(CH_3)$	CG331	0.365	0.326
Methanol				$H(CH_3)$	HGA3	0.239	0.100
$C(CH_3)$	CG331	0.365	0.326	$C(CH_2)$	CG321	0.358	0.234
$H(CH_3)$	HGA3	0.239	0.100	$H(CH_2)$	HGA2	0.239	0.146
O(O)	OG311	0.314	0.804	O(O)	OG301	0.294	0.428
H(H)	HGP1	0.04	0.192	**Toluene**			
Acetone				$C(C_6H_5)$	CG2R61	0.355	0.293
$C(CH_3)$	CG331	0.365	0.326	$H(C_6H_5)$	HGR61	0.242	0.126
$H(CH_3)$	HGA3	0.239	0.100	$C(CH_3)$	CG331	0.365	0.326
C(CO)	CG2O5	0.356	0.377	$H(CH_3)$	HGA3	0.239	0.100
O(CO)	OG2D3	0.303	0.209				