Supplementary Material

Impact of Structural Functionalization, Pore Size, and Presence of Extra-Framework Ions on the Capture of Gaseous I_2 by MOF Materials

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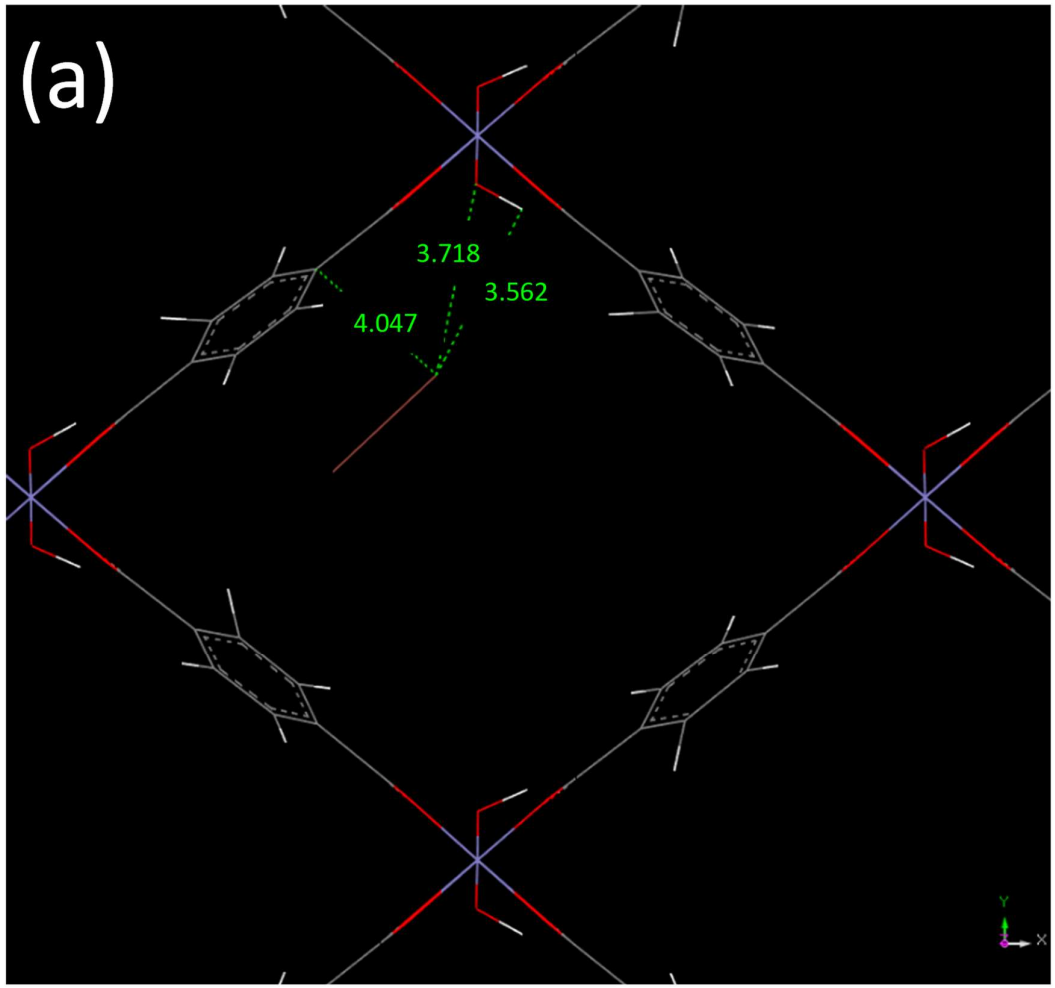
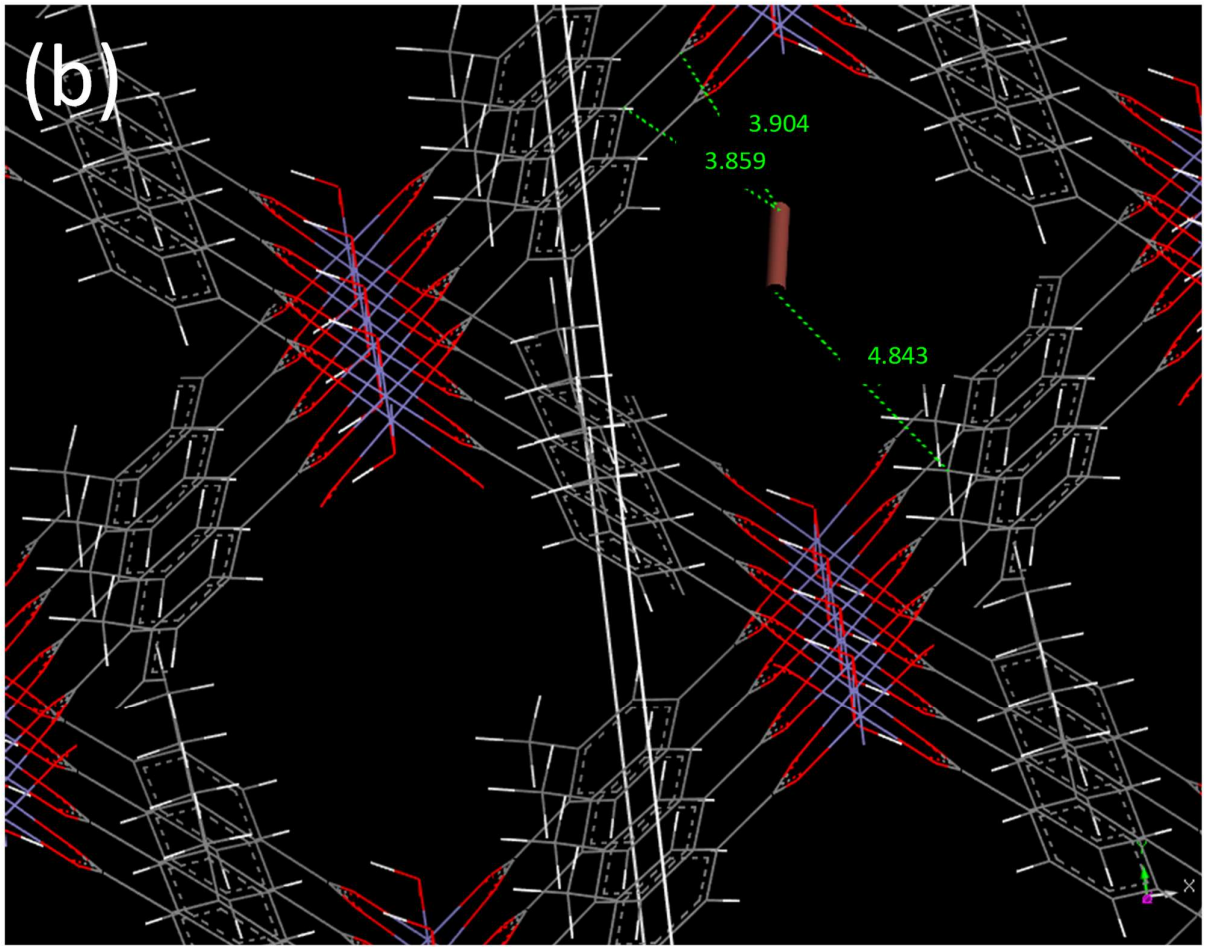
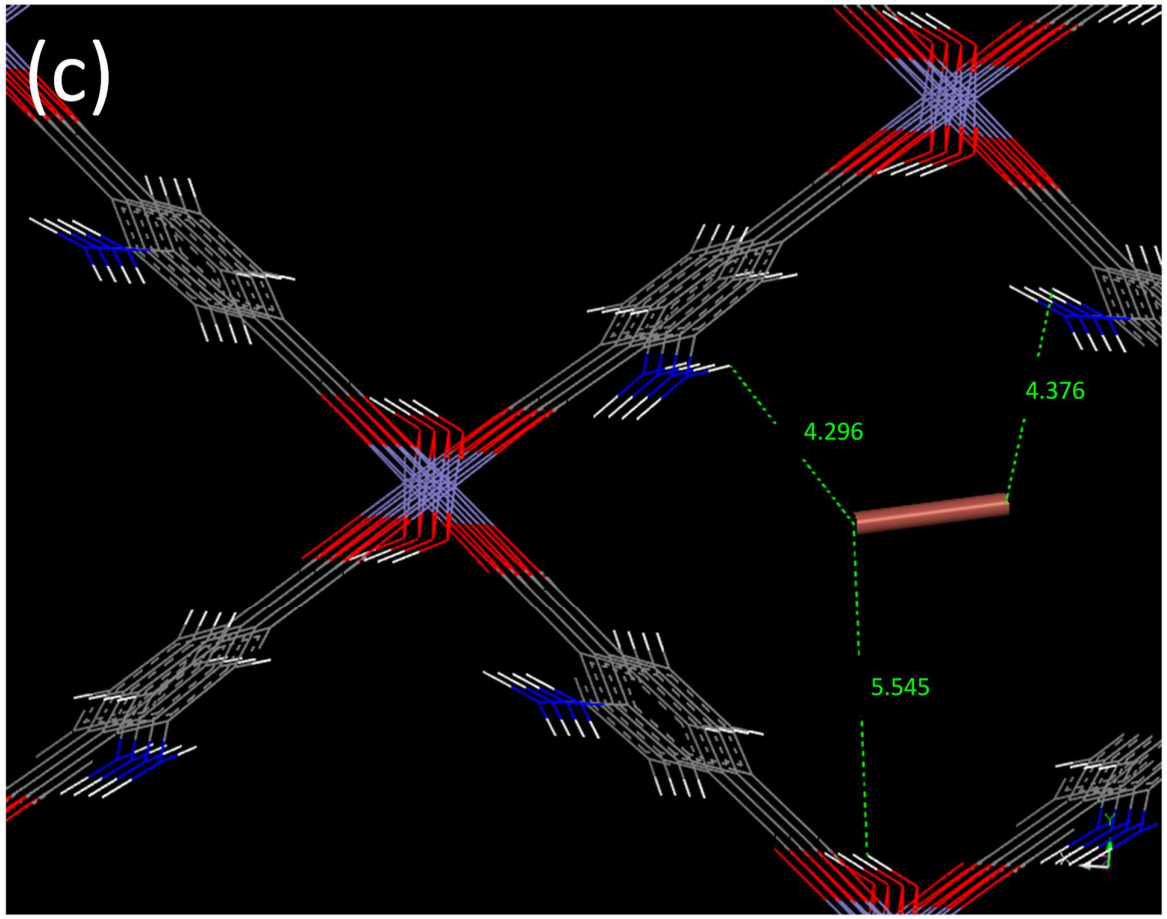
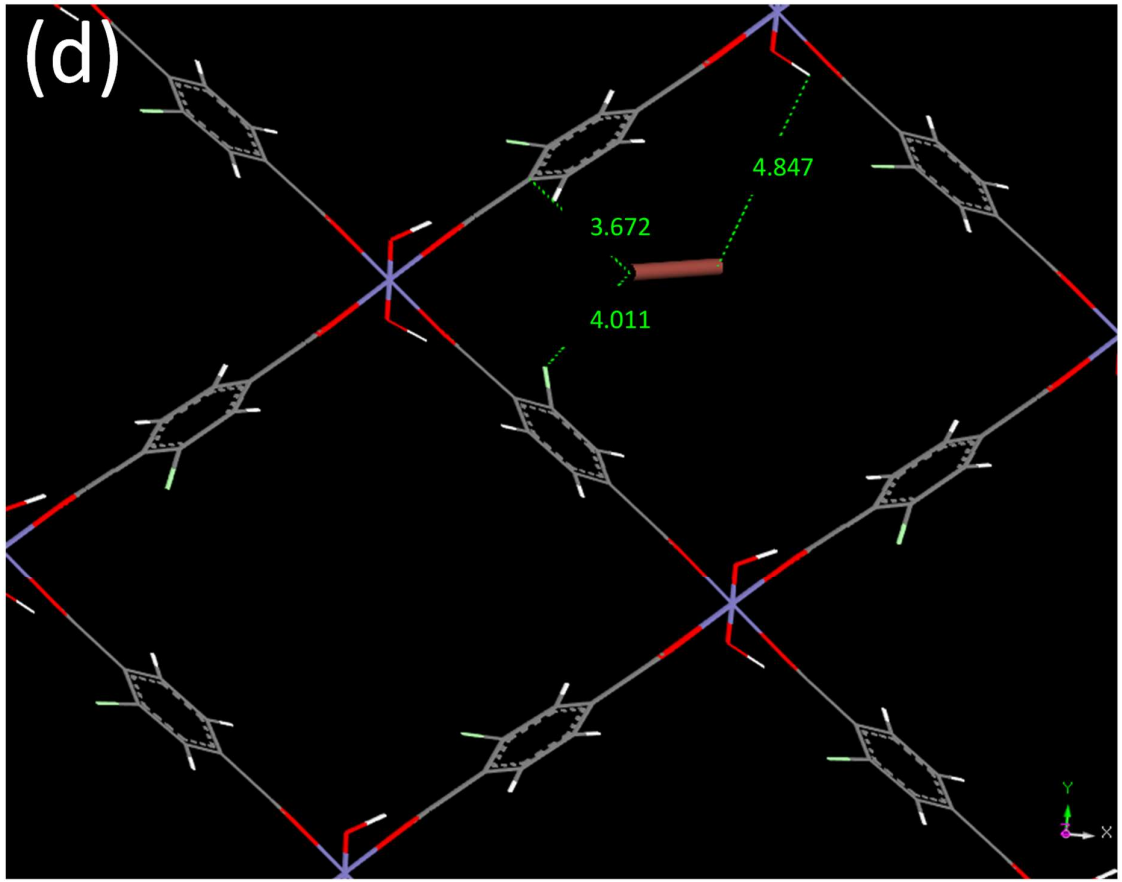

(a)
3.718
3.562
4.047
Y
X


(b)
3.904
3.859
4.843


(c)
4.296
4.376
5.545


(d)
4.847
3.672
4.011
Y
X

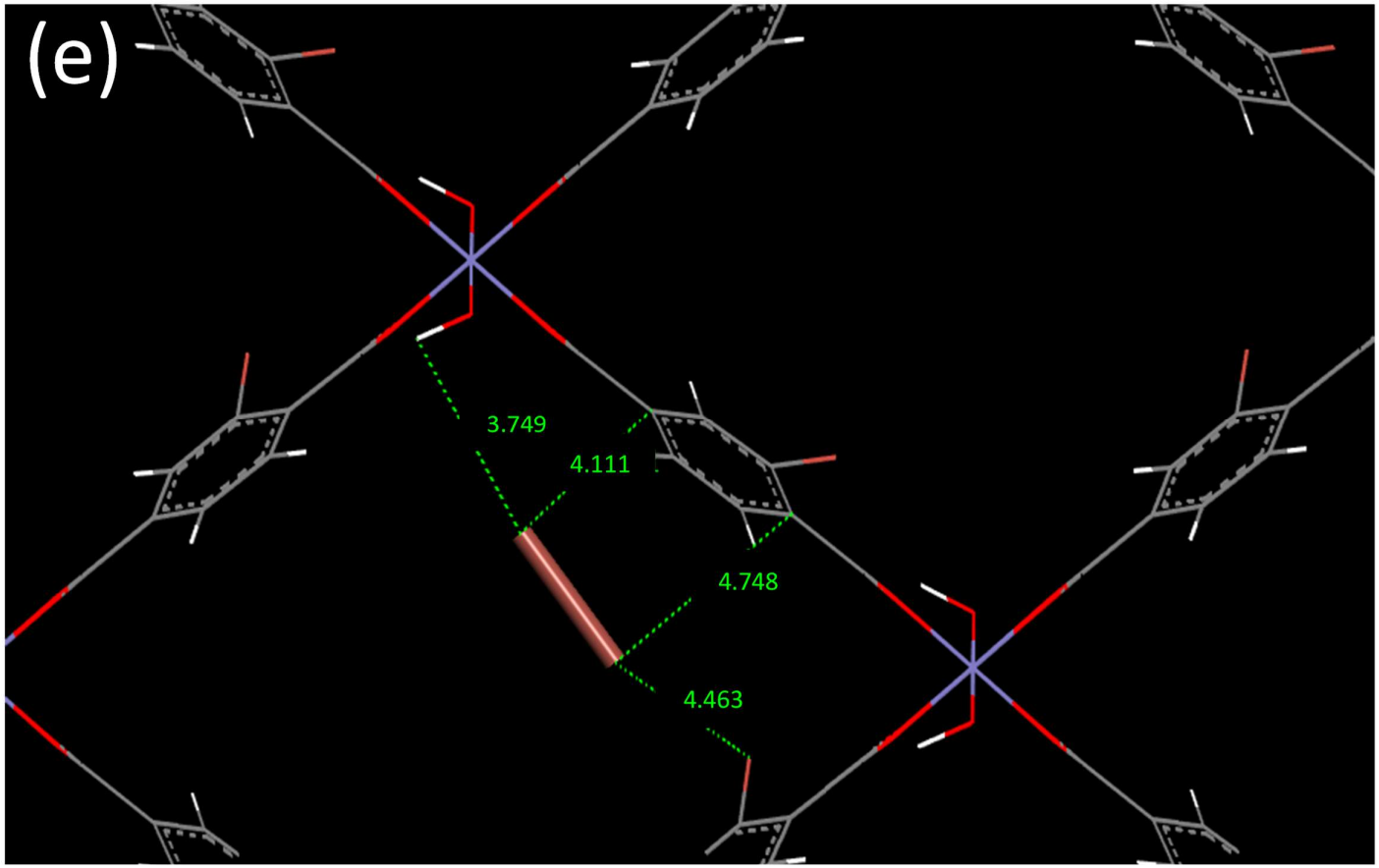
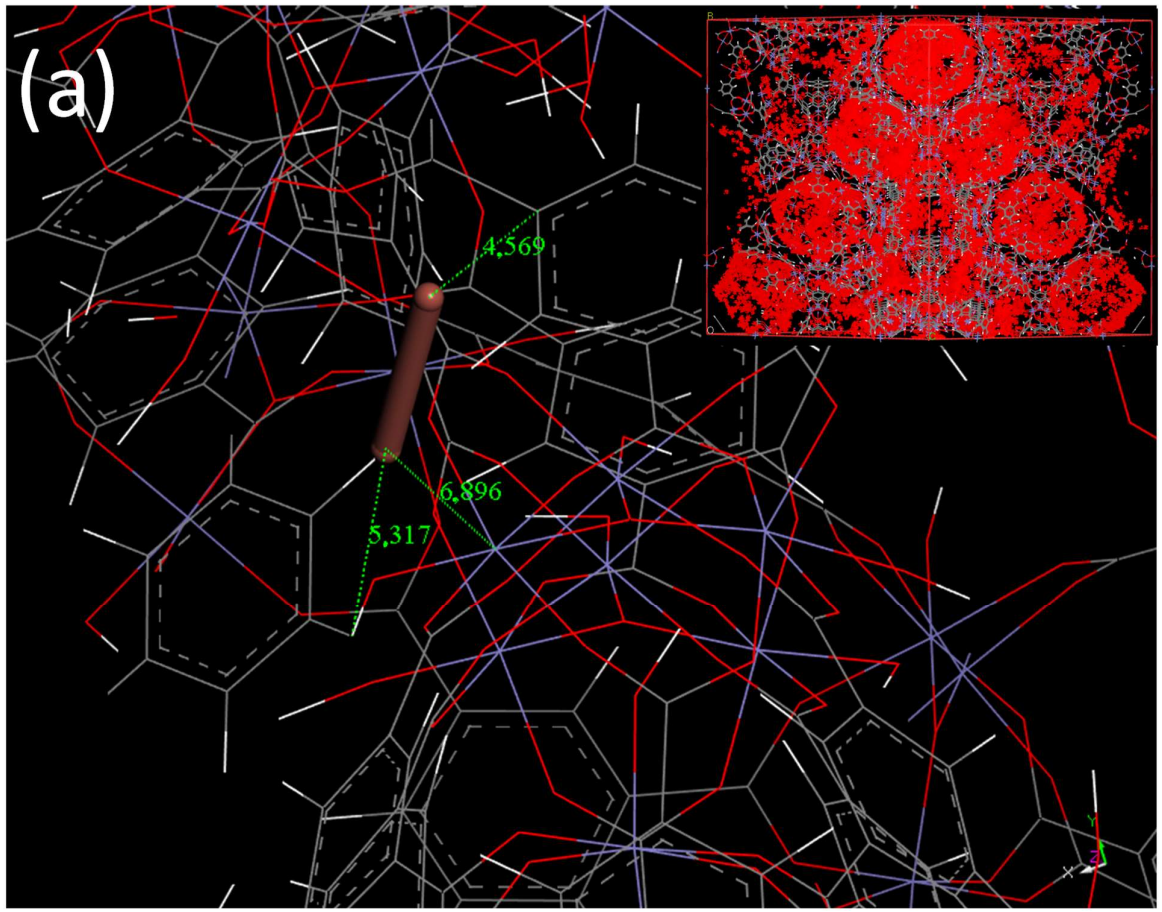
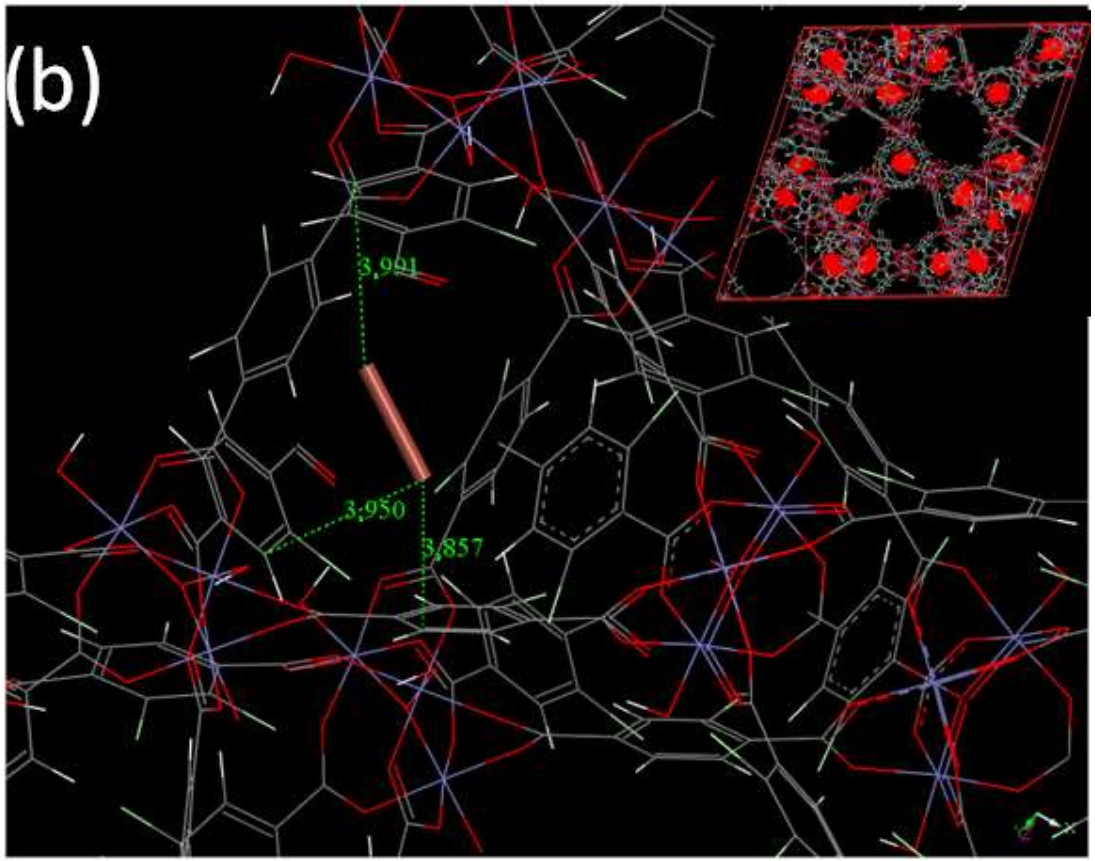
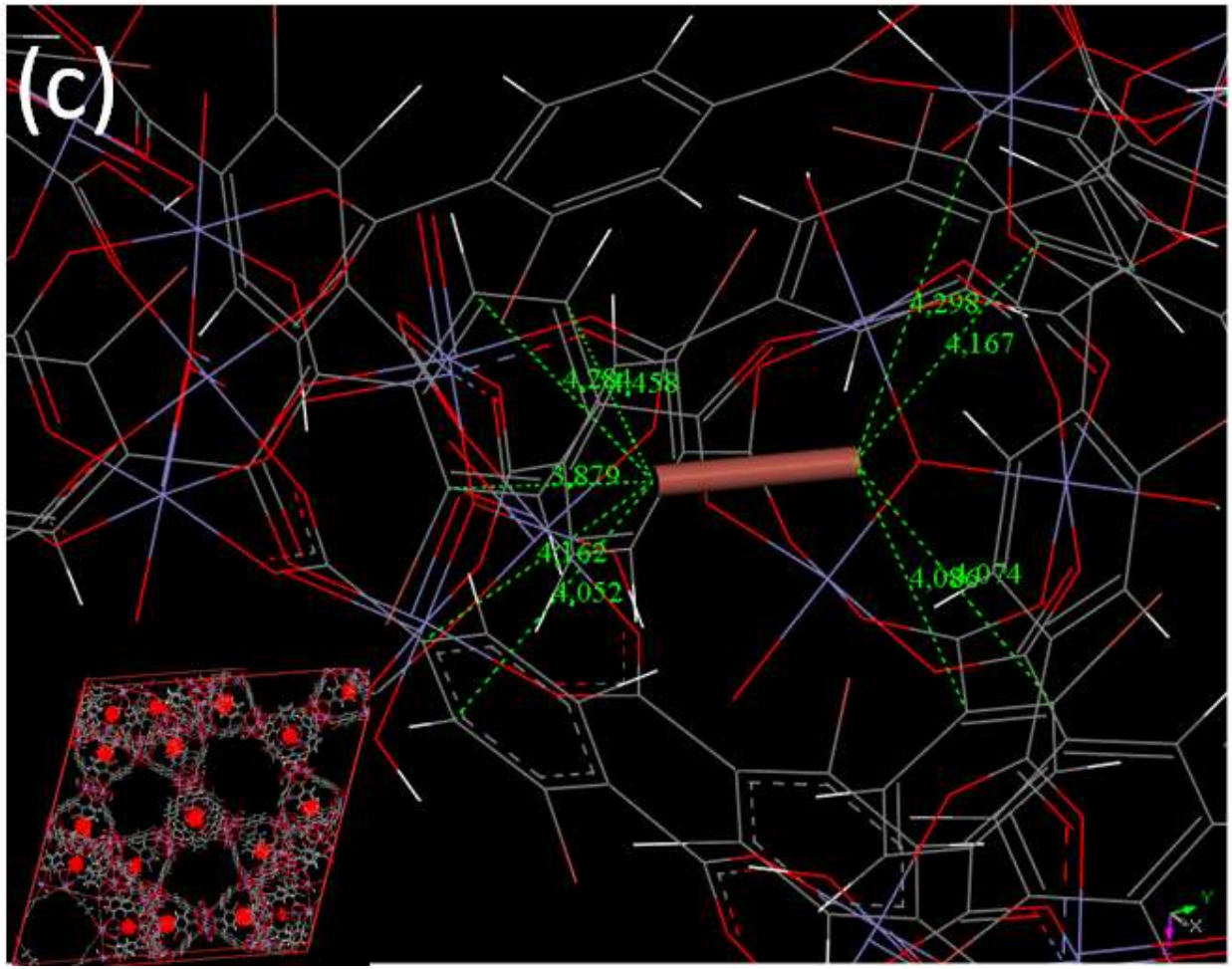
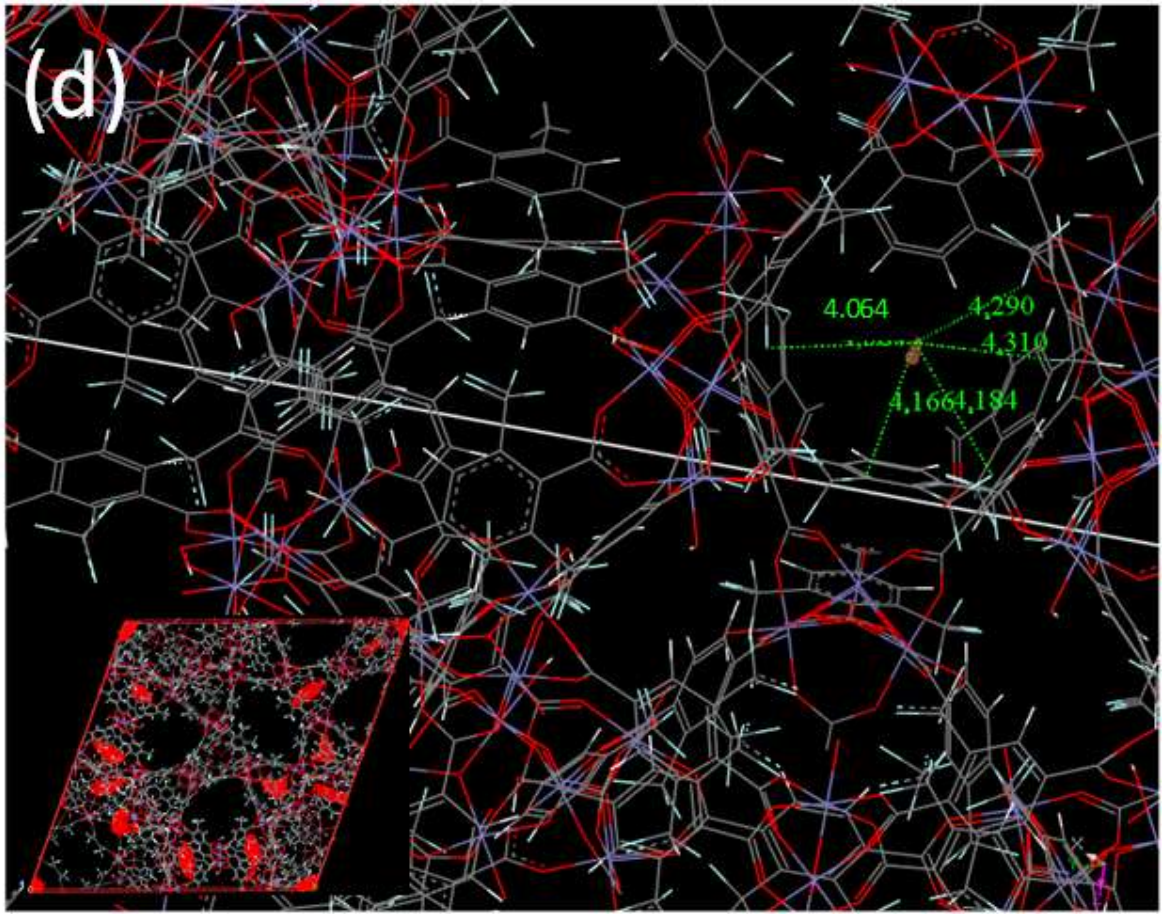


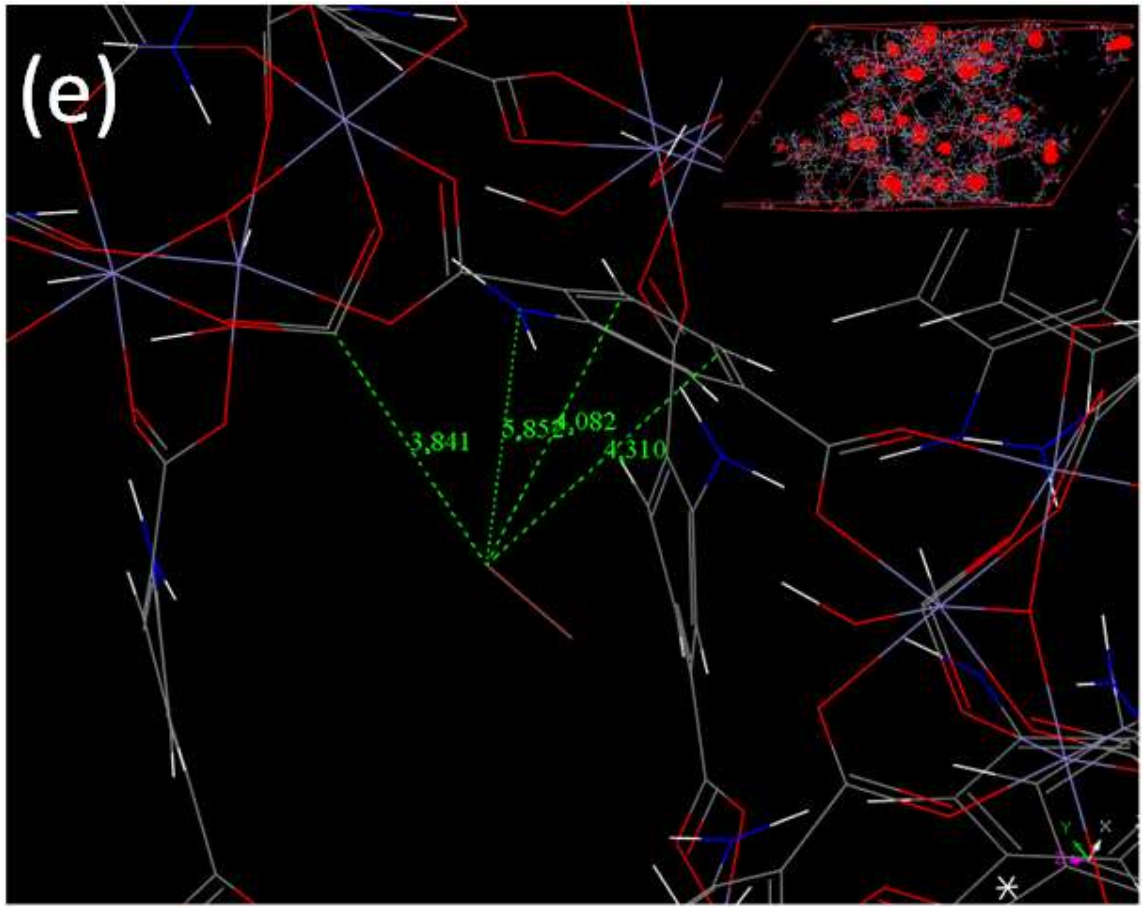
Figure S1. Molecular conformations of the first I_2 molecule adsorbed onto MOF structures belonging to the MIL-53 series functionalized by: (**a**) H, (**b**) CH_3, (**c**) NH_2, (**d**) Cl, (**e**) Br, as obtained based on the Monte Carlo simulations.

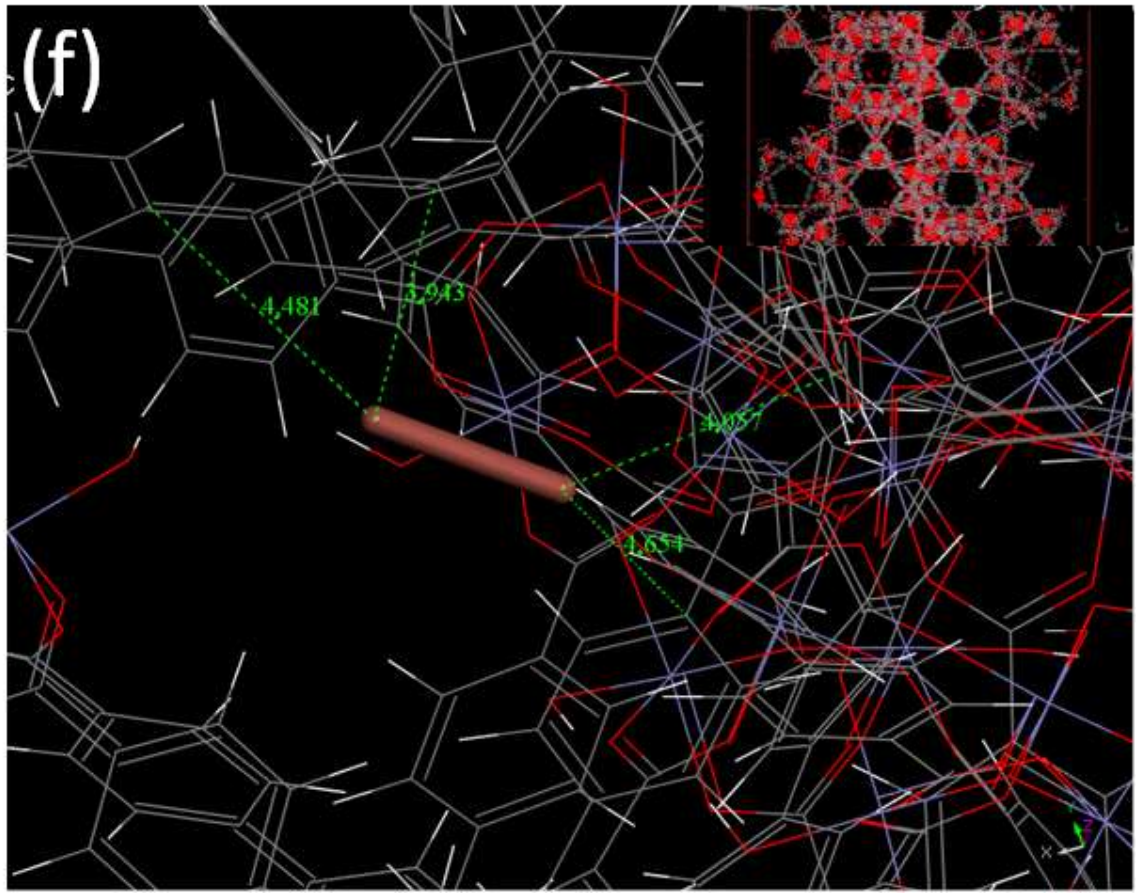

(a)
4,569
6,896
5,317


(b)
3,991
3,950
3,857


(c)
4.298
4.167
4.458
3.879
4.162
4.052
4.086
4.074


(d)
4.064
4,290
4,310
4,166
4,184


(e)
3,841
5,852
4,082
4,310


(f)
4.481
3.943
4.654

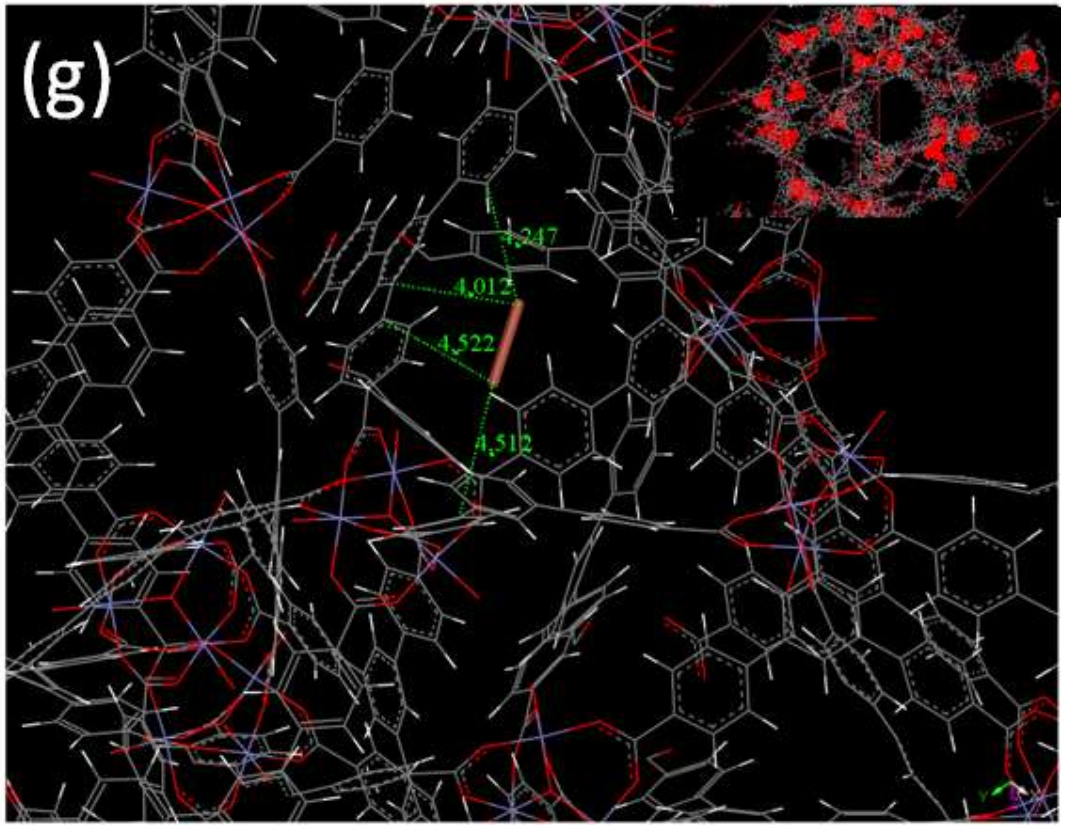
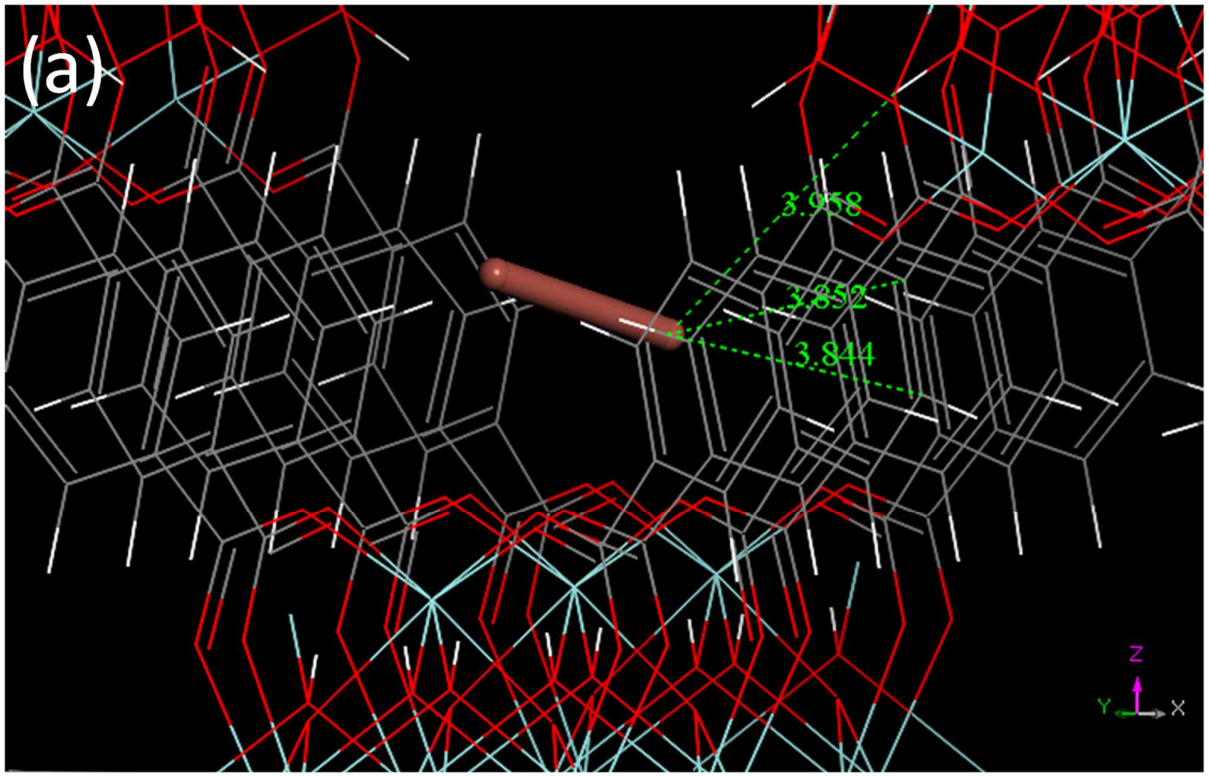
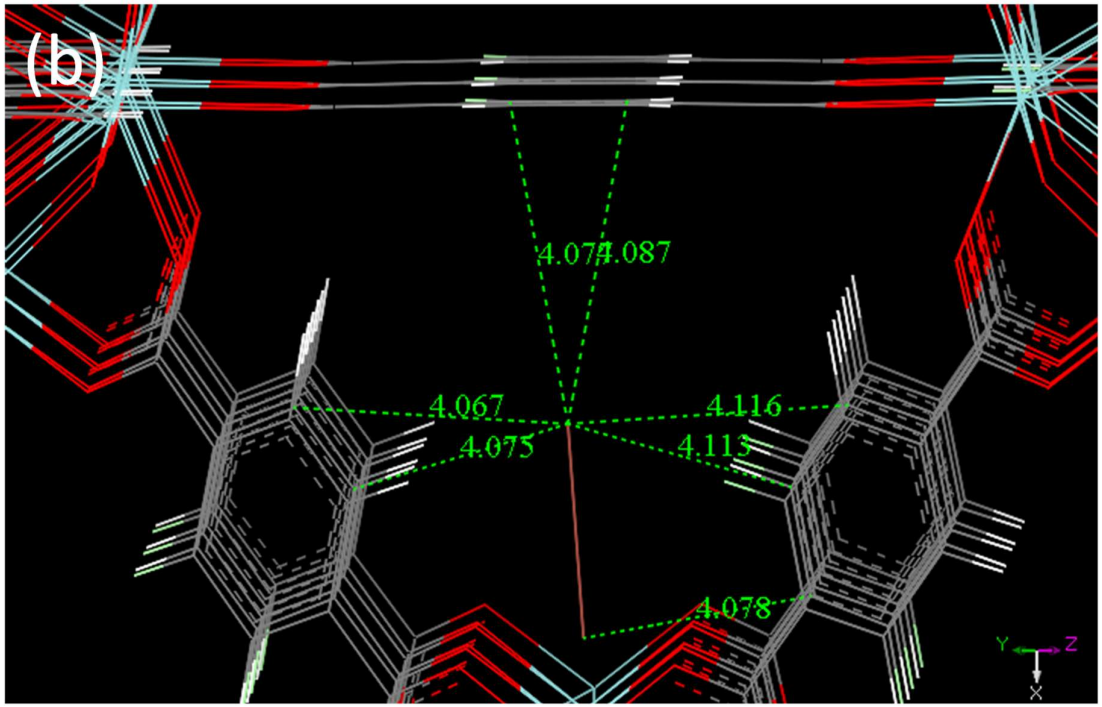
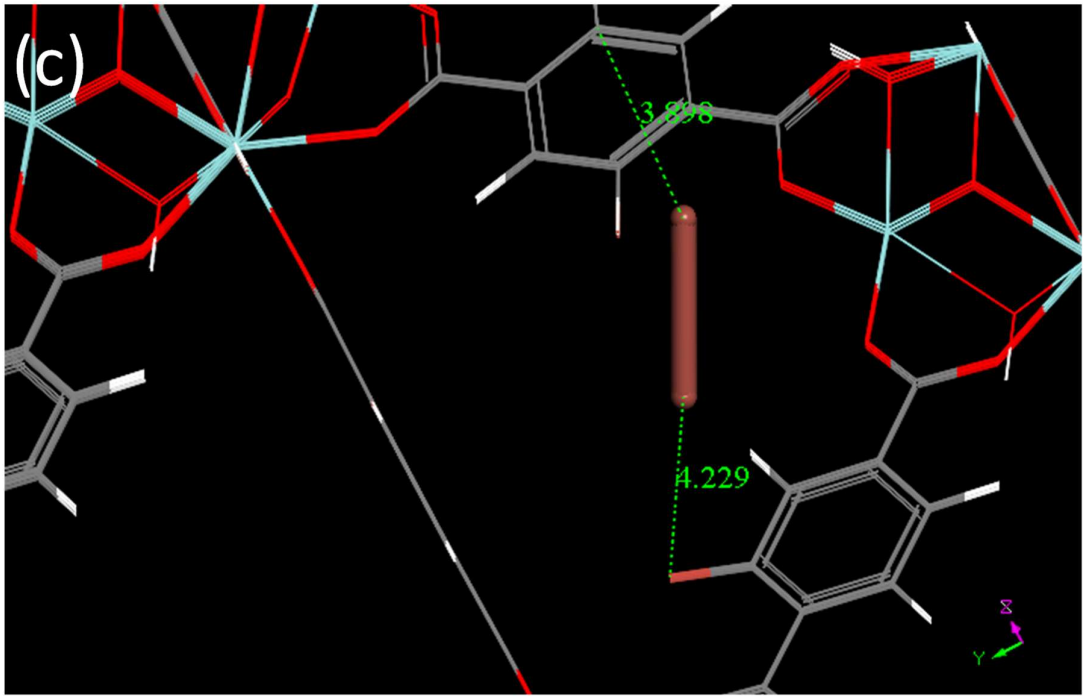
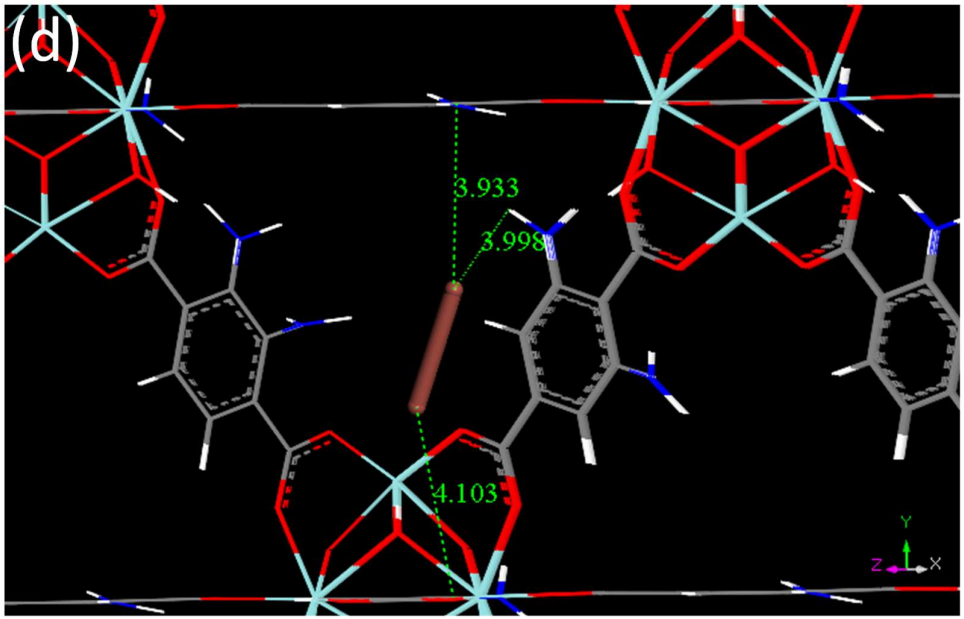


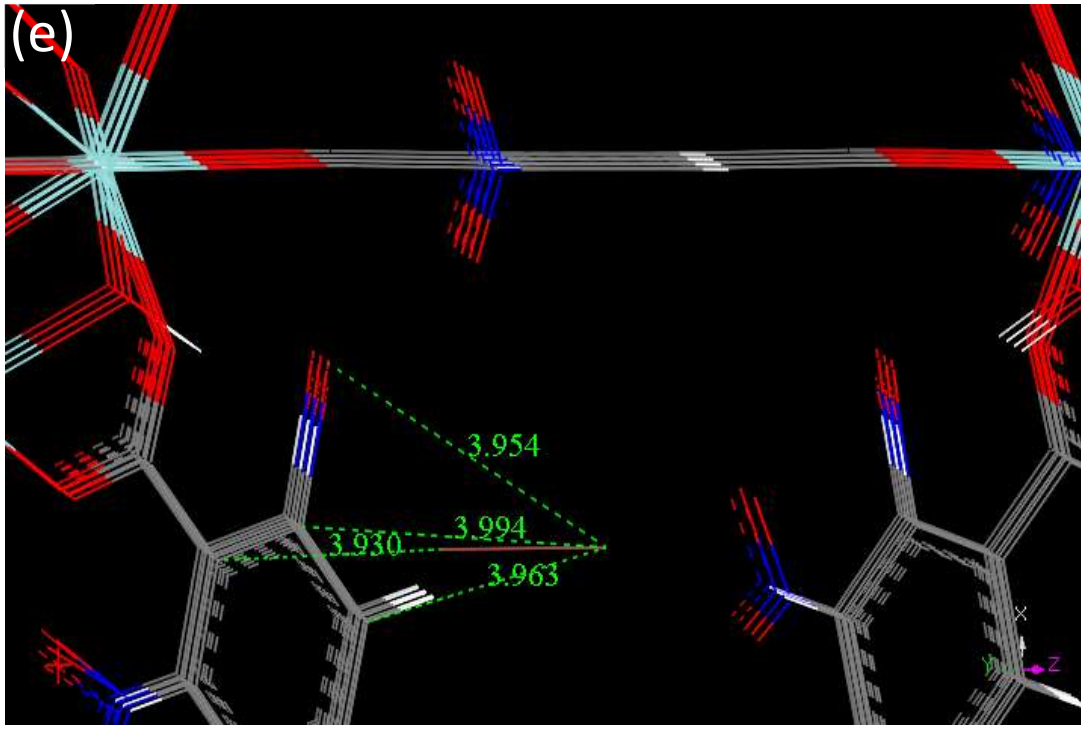
Figure S2. Molecular conformations of the first I_2 molecule adsorbed onto MOF structures belonging to the MIL-100/101 series: (**a**) MIL-100, (**b**) MIL-101-Cl, (**c**) MIL-101-Br, (**d**) MIL-101-2CF_3, (**e**) MIL-101-NH_2, (**f**) MIL-101-biphenyl, (**g**) MIL-100-BTB, as obtained based on the Monte Carlo simulations. At the corner of the picture, the density plot (red points) to localize the main adsorption sites is given for each sample.

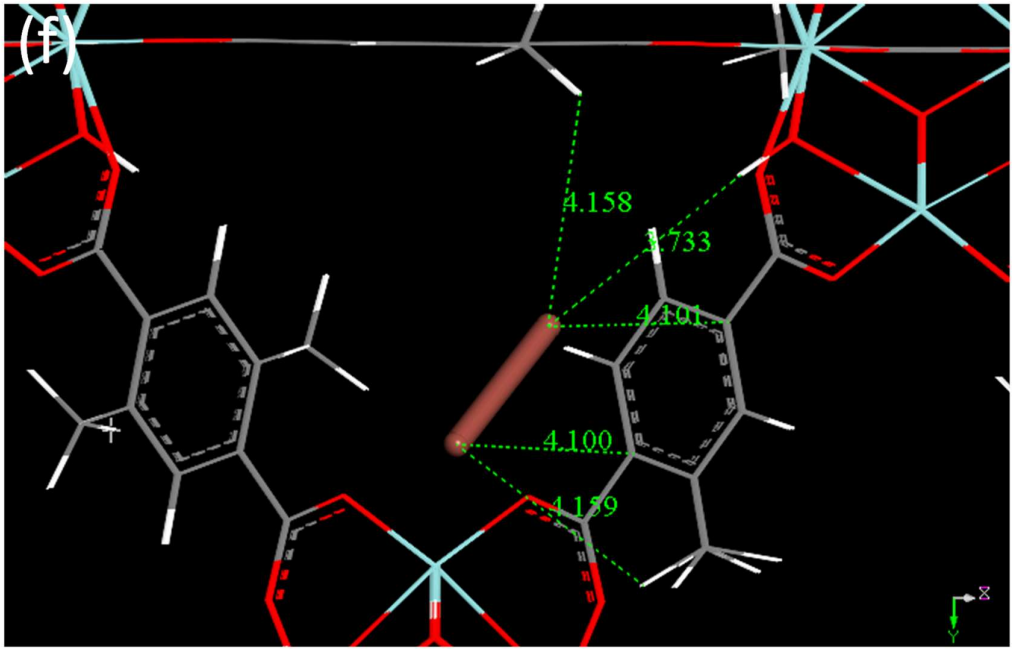

(a)
3.858
3.852
3.844
Z
Y
X


(b)
4.074
4.087
4.067
4.116
4.075
4.113
4.078
Y
Z
X


(c)
3.878
4.229
Z
Y


(d)
3.933
3.998
4.103
Y
Z
X


(e)
3.954
3.930
3.994
3.963
X
Z


(f)
4.158
3.733
4.101
4.100
4.159

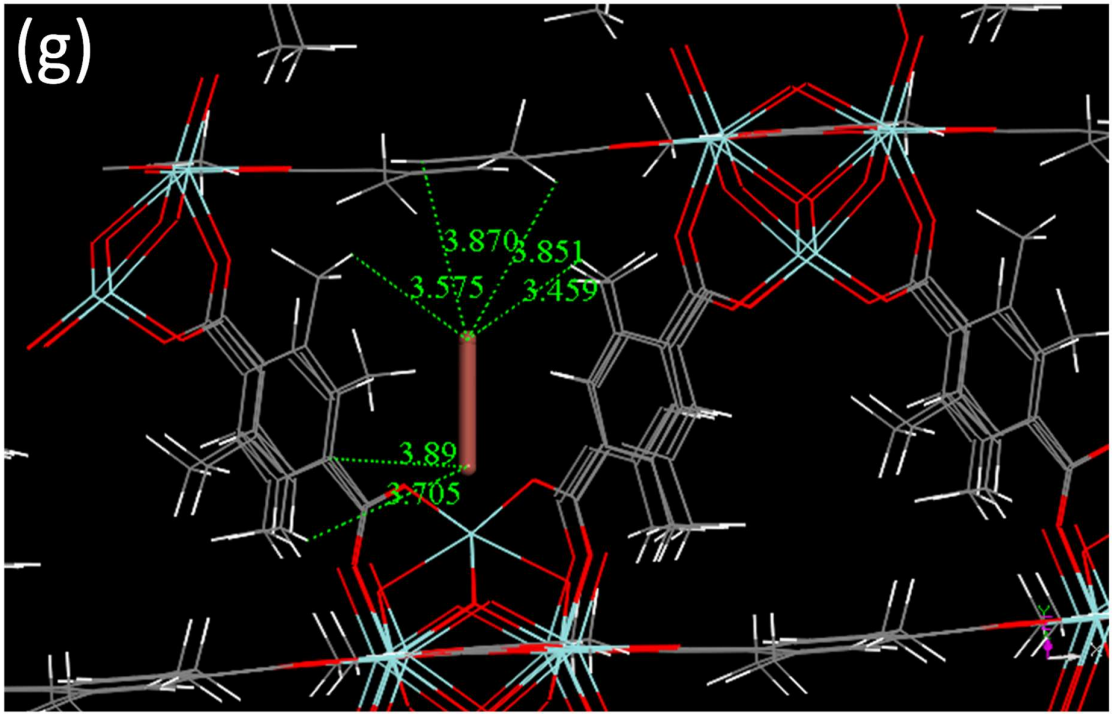


Figure S3. Molecular conformations of the first I_2 molecule adsorbed onto MOF structures belonging to the UiO-66 series: (**a**) H, (**b**) Cl, (**c**) Br, (**d**) NH_2, (**e**) NO_2, (**f**) CH_3, (**g**) $2CH_3$, as obtained based on the Monte Carlo simulations

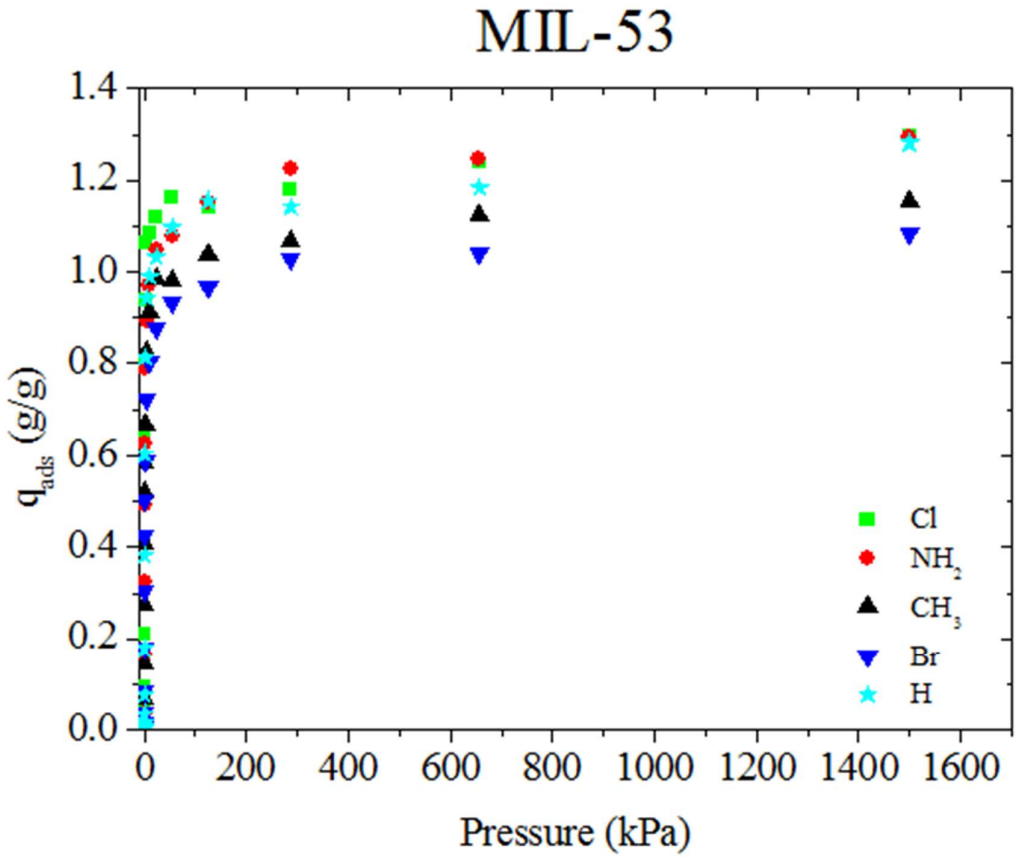


Figure S4. Adsorption isotherms for I_2 onto MOF structures belonging to the MIL-53 series, as calculated based on the Monte Carlo simulations

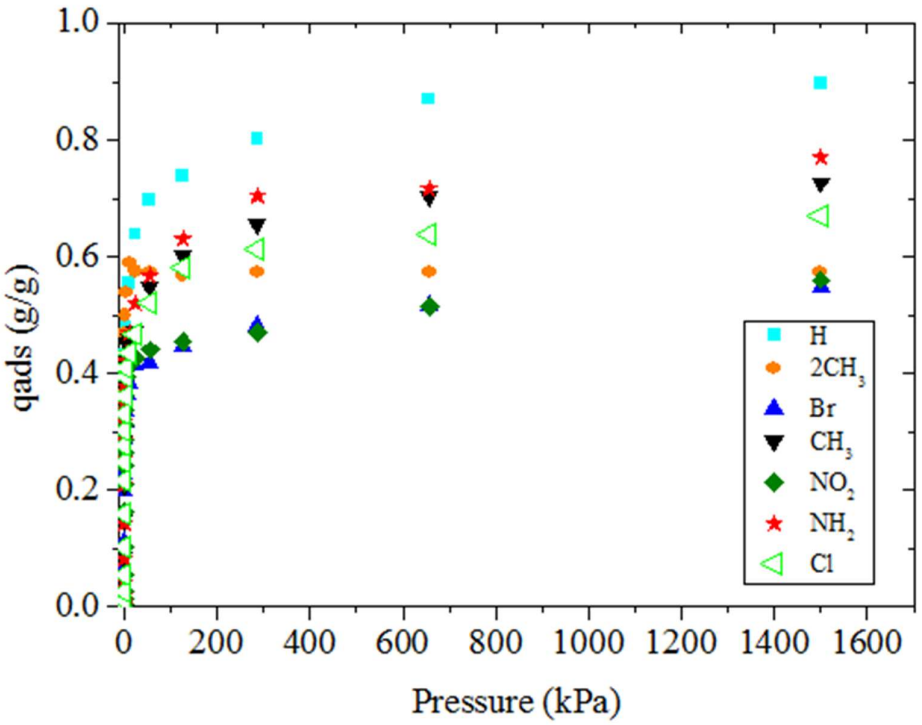


Figure S5. Adsorption isotherms for I_2 onto MOF structures belonging to the UiO-66 series, as calculated based on the Monte Carlo simulations

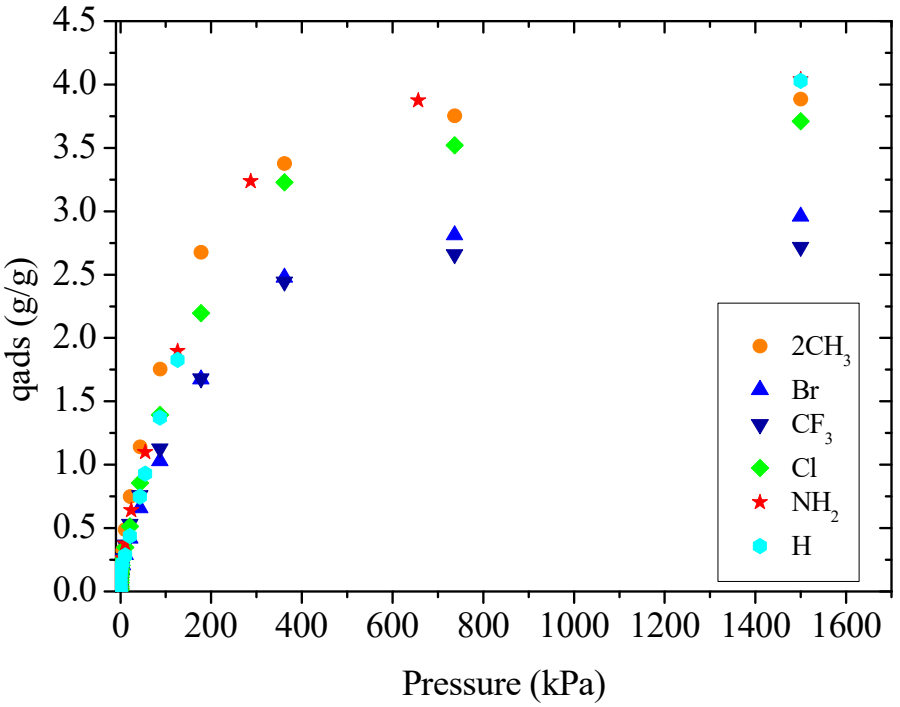


Figure S6. Adsorption isotherms for I_2 onto MOF structures belonging to the MIL-101 series, as calculated based on the Monte Carlo simulations

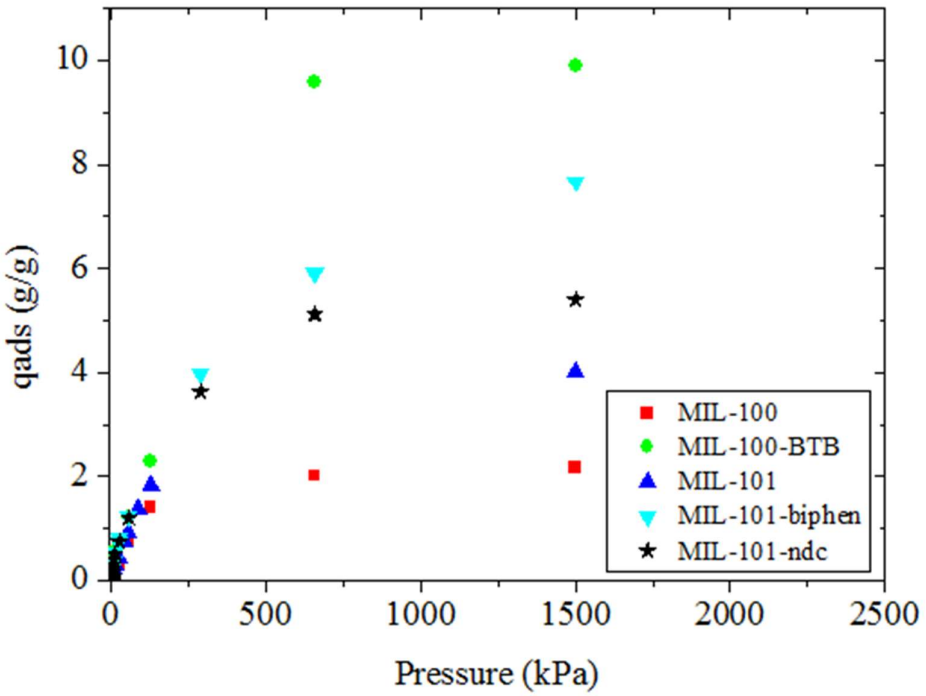


Figure S7. Adsorption isotherms for I_2 onto MOF structures belonging to the modified MIL-100/MIL-101 solids, as calculated based on the Monte Carlo simulations.

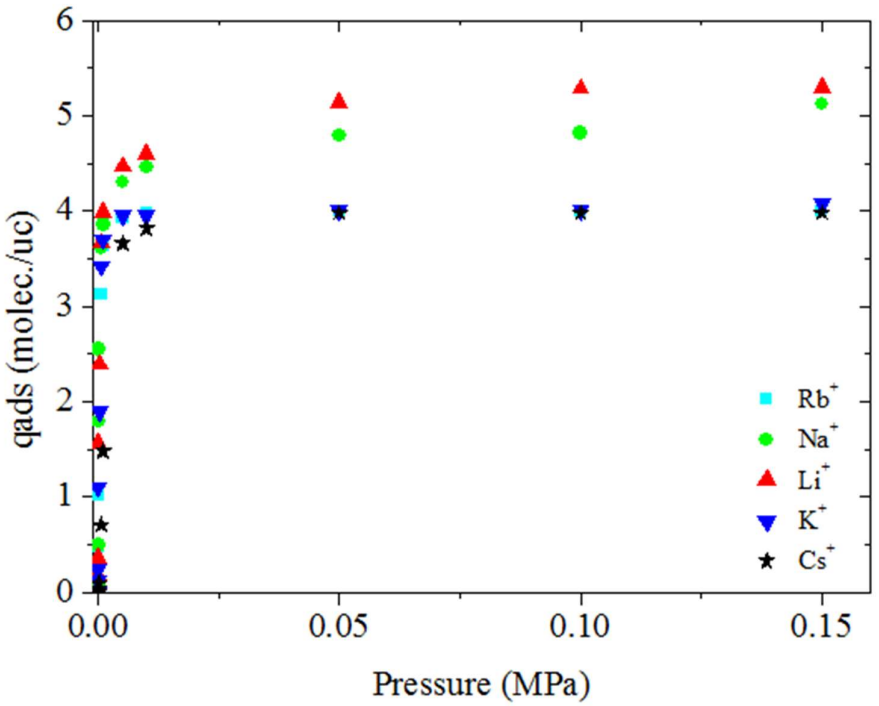


Figure S8. Adsorption isotherms for I_2 onto MOF structures belonging to the cation-saturated Zn-BTeC family, as calculated based on the Monte Carlo simulations.

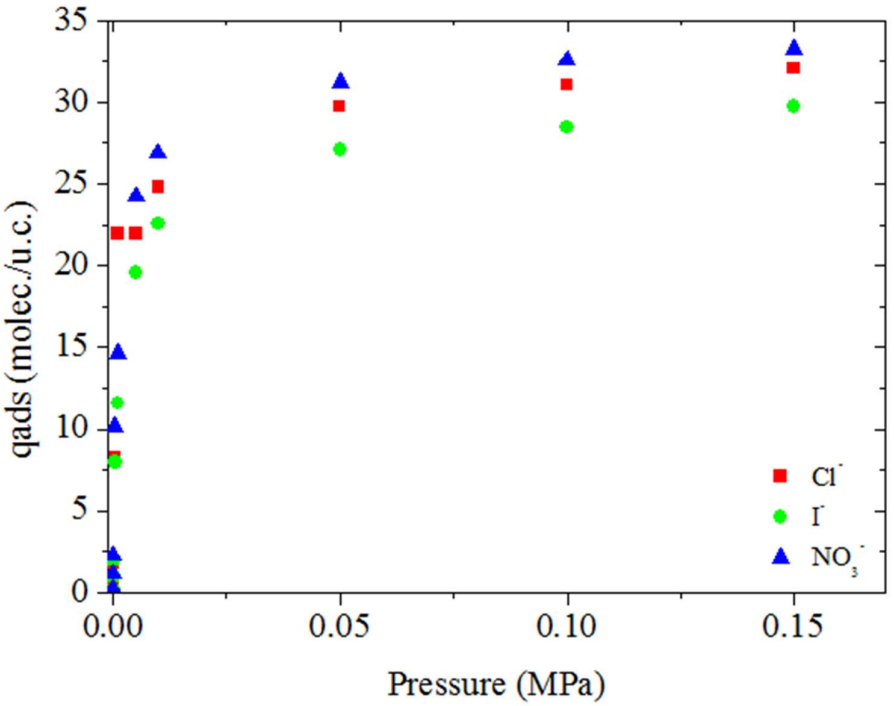


Figure S9. Adsorption isotherms for I_2 onto MOF structures belonging to the anion-saturated MIL-127, as calculated based on the Monte Carlo simulations.