Electronic Supplementary Information

Tailoring of the Electronic Property of Zn-BTC Metal-organic Framework via Ligand Functionalization: An ab-initio Investigation

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BTC MOFs structural comparisons

Table 1: Calculated structural information in comparison to experimental results and other MOF structures. $< M - M >$ is the distances between the metal centers at the SBU while $< M - O_t >$ refers to the average metal-oxygen bond length at the metal centers in the SBU.

MOF system	Metal site	Cell parameters (Å)	Bond lengths (Å)		Ref.
		$a = b = c$	$M - M$	$< Zn - O_t >$	
Zn-BTC	saturated	27.02	3.38	1.86	this work
Cu-BTC.H_2O	saturated	26.34	2.63		[1]
NH_2-Zn-BTC	saturated	27.72	2.46	1.86	this work
NH_2-Cu-BTC	saturated	26.58	2.63	2.18	[2]

Electronic information

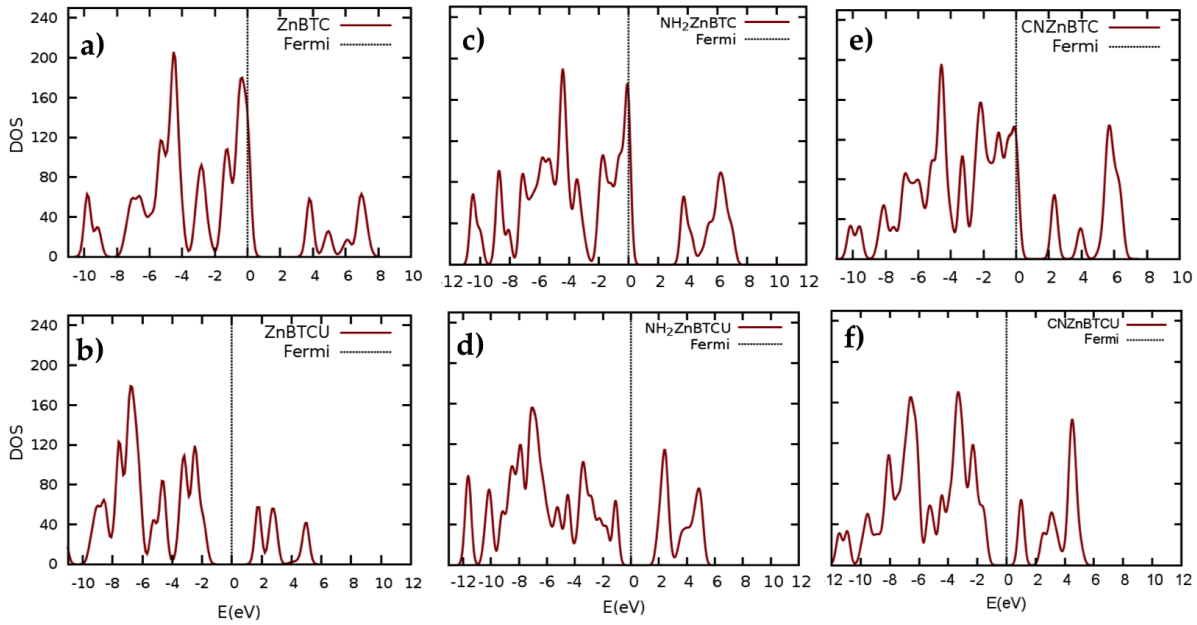

Figure 1: (color online) Calculated density of states (DOS) for pristine a) saturated b) unsaturated, amino-functionalized c) saturated d) unsaturated, and cyano-functionalized e) saturated f) unsaturated SBU Zn-BTC MOFs.

References

[1] M. K. Bhunia, J. T. Hughes, J. C. Fettinger, and A. Navrotsky. Thermochemistry of paddle wheel mofs: Cu-hkust-1 and zn-hkust-1. Langmuir, 29(25):8140?8145, 2013.
[2] K. Peikert, F. Hoffmann, and M. Froba. Amino substituted cu 3 (btc) 2: a new metal-organic framework with a versatile functionality. Chemical Communications, 48(91):11196?11198, 2012.