Supporting Information

Density Functional Theory Study of Li-Functionalized Nanoporous R-Graphyne-Metal-Organic Frameworks for Reversible Hydrogen Storage

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TABLE S1: Bond distances between functionalized Li atoms and R-graphyne unit (Li-G^R), Li atoms and adsorbed H_2 molecules (Li-H), and inter-atomic distance between adsorbed hydrogen atoms (H-H).

System	Li-G^R (Å)	Li-H (Å)	H-H (Å)
G^R-MOF-Li_8	2.257	-	-
G^R-MOF-Li_8-$8H_2$	2.220	1.990	0.771
G^R-MOF-Li_8-$16H_2$	2.307	1.986	0.771
G^R-MOF-Li_8-$24H_2$	2.277	2.008	0.762
G^R-MOF-Li_8-$32H_2$	2.332	2.037	0.768