Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Methane Capture at Room Temperature: Adsorption on δ-MoC and β-Mo_2C Molybdenum Carbides (001) Surfaces

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Table S1: Adsorption structural data and energy values for methane molecule adsorbed on β-Mo_2C(001) surfaces. IS and FS stand for initial and final structures, respectively, energies are in eV, distances in Å, and charges in number of electrons.

IS	FS	E_{ads}	E_{ads}+vdW	%vdW	ΔC-H_s	ΔC-H_f	ΔQ (C)	ΔQ(H_s)	ΔQ(H)
					0.006			0.00	
β(C)-H_3(hC)	H_3(hC)	-0.05	-0.29	82.8	0.006	0.005	-0.06	-0.03	0.00
					0.005			0.09	
						0.002			-0.01
β(C)-H_1(hC)	H_1(hC)	-0.04	-0.24	83.3	0.014	0.003	-0.04	0.07	-0.01
						0.002			0.00
β(C)-H_2(hC)	H_2(hC)	-0.05	-0.29	82.8	0.002	0.002	-0.27	0.06	0.06
					0.002	0.002		0.08	0.08
β(Mo)-H_2(hC^2)	H_2(tMo)	-0.11	-0.39	71.8	0.027	0.002	-0.10	0.09	-0.01
					0.029	0.001		0.05	0.04
β(Mo)-H_3(tMo)	H_2(tMo)[a]	-0.03	-0.39	92.3	0.027	0.002	-0.10	0.09	-0.01
					0.029	0.001		0.05	0.04
β(Mo)- H_1(hMo)	H_2(tMo)[a]	-0.03	-0.39	92.3	0.027	0.002	-0.10	0.08	-0.01
					0.029	0.001		0.05	0.03

[a]These geometries are obtained only when vdW correction is included.

Table S2: Adsorption data and energy values for methane adsorption on δ-MoC(001) surfaces. IS and FS stand for initial and final structures, respectively, energies are in eV, distances in Å, and charges in number of electrons.

IS	FS	E_{ads}	E_{ads}+vdW	%vdW	ΔC-H_s	ΔC-H_f	ΔQ (C)	ΔQ (H_s)	ΔQ (H)
δ-H_3(h)	δ-H_3(h)	-0.54	-0.92	41.3	0.006 0.003 0.003	0.004	-0.03	0.00 0.01 0.03	-0.02
δ-H_3(tC)	δ-H_3(tC)	-0.54	-0.90	40.0	0.004 0.004 0.004	0.004	-0.02	-0.03 0.00 0.03	0.01
δ-H_2(tMo)	δ-H_2(tMo)	-0.54	-0.96	43.8	0.007 0.005	0.003 0.003	0.01	-0.05 0.01	-0.01 0.02
δ-H_3(tMo)	δ-H_3(tMo)	-0.55	-0.95	42.1	0.004 0.005 0.004	0.004	-0.02	-0.02 0.01 0.05	-0.03