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Supplementary Information

Probing Topological Electronic Effects in Catalysis: Thiophene Adsorption on NiMoS and CoMoS Clusters

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Table S1. DFT distributed multipole analysis at selected sites of the $Ni_3Mo_{13}S_{32}$ cluster (Q_0 charge, Q_1 dipole and Q_2 quadrupole). All values are in atomic units (ea_0^k for Q_k). Atom notation follows from Figures 1 and 2. For dipole values (Q_1): 1 a. u. (ea_0) = 2.5417 D

	$Ni_{c,IV}$	$Ni_{e,IV}$	$S_{c,II}$	$S_{o,III}$	$Mo_{o,VI}$	$Mo_{i,VI}$
Q_0	–0.24	–0.26	–0.19	–0.10	0.93	0.84
Q_1	0.27	0.19	0.31	0.33	0.28	0.20
Q_2	0.45	0.76	1.07	0.88	0.64	0.59

Table S2. DFT distributed multipole analysis at selected sites of the $Co_3Mo_{13}S_{32}$ cluster (Q_0 charge, Q_1 dipole and Q_2 quadrupole). All values are in atomic units (ea_0^k for Q_k). Atom notation follows from Figures 1 and 2

	$Co_{c,IV}$	$Co_{e,IV}$	$S_{c,II}$	$S_{o,III}$	$Mo_{o,VI}$	$Mo_{i,VI}$
Q_0	–0.19	–0.15	–0.21	–0.14	0.90	0.87
Q_1	0.38	0.39	0.33	0.33	0.26	0.18
Q_2	0.42	0.60	1.00	0.71	0.59	0.40

Table S3. DFT distributed multipole analysis at selected sites of the $Mo_{16}S_{32}$ cluster (Q_0 charge, Q_1 dipole and Q_2 quadrupole). All values are in atomic units (ea_0^k for Q_k). Atom notation follows from Figures 1 and 2

	$Mo_{c,IV}$	$Mo_{e,IV}$	$S_{c,II}$	$S_{o,III}$	$Mo_{o,VI}$	$Mo_{i,VI}$
Q_0	0.81	0.73	–0.39	–0.43	0.78	0.73
Q_1	0.07	0.13	0.16	0.29	0.15	0.05
Q_2	0.84	1.00	0.81	0.50	0.52	0.19

Table S4. DFT distributed multipole analysis for the thiophene molecule (Q_0 charge, Q_1 dipole and Q_2 quadrupole). All values are in atomic units (ea_0^k for Q_k). Carbon atom numbers follow from Figure 2

	S	C1	C2	C3	C4
Q_0	0.63	–0.34	–0.07	–0.07	–0.34
Q_1	1.19	0.45	0.03	0.03	0.45
Q_2	2.03	1.68	1.32	1.32	1.68

Table S5. DFT distributed multipole analysis at selected sites of the thiophene plus $Ni_3Mo_{13}S_{32}$ system (Q_0 charge, Q_1 dipole and Q_2 quadrupole). All values are in atomic units (ea_0^k for Q_k). Atom numbers follow from Figure 2

	Atom															
	$Ni^*_{c,iv}$	$Ni_{e,iv}$	$Ni_{c,iv}$	$S^*_{c,II}$	$S^*_{o,iii}$	$S_{o,III}$	$S_{c,II}$	$Mo^*_{o,VI}$	$Mo^*_{i,VI}$	$Mo_{i,VI}$	$Mo_{o,VI}$	S	C1	C2	C3	C4
Q_0	–0.22	–0.29	–0.25	–0.19	–0.08	–0.08	–0.19	0.93	0.85	0.84	0.93	0.70	–0.32	–0.07	–0.11	–0.36
Q_1	0.52	0.17	0.27	0.40	0.39	0.36	0.33	0.28	0.20	0.20	0.28	1.04	0.43	0.07	0.16	0.45
Q_2	0.58	0.92	0.49	1.15	0.76	0.93	1.06	0.58	0.51	0.61	0.65	1.79	1.57	1.39	1.16	1.47

Table S6. DFT distributed multipole analysis at selected sites of the thiophene plus $Co_3Mo_{13}S_{32}$ system (Q_0 charge, Q_1 dipole and Q_2 quadrupole). All values are in atomic units (ea_0^k for Q_k). Atom numbers follow from Figure 2

	Atom															
	$Co^*_{c,iv}$	$Co_{e,iv}$	$Co_{c,iv}$	$S^*_{c,II}$	$S^*_{o,iii}$	$S_{o,III}$	$S_{c,II}$	$Mo^*_{o,VI}$	$Mo^*_{i,VI}$	$Mo_{i,VI}$	$Mo_{o,VI}$	S	C1	C2	C3	C4
Q_0	–0.18	–0.32	–0.20	–0.15	–0.03	–0.03	–0.17	0.89	0.81	0.82	0.90	0.73	–0.29	–0.05	–0.05	–0.38
Q_1	0.54	0.22	0.39	0.38	0.36	0.37	0.37	0.30	0.22	0.25	0.28	0.91	0.41	0.05	0.13	0.44
Q_2	0.91	0.80	0.49	1.21	0.80	0.93	1.06	0.51	0.51	0.61	0.60	1.39	1.47	1.33	1.28	1.27

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