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Effect of Oxygen Termination on the Interaction of First Row Transition Metals with M_2C MXenes and the Feasibility of Single-Atom Catalysts†

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Adatom		site	E_{ads} (eV)	h (Å)	ΔQ (e)	E_{diff}	E_{bar}
Sc	PBE	**H_C**	**-6.292**	**1.023**	**1.816**	**2.17**	
	PBE-D3		**-6.666**	**1.019**	**1.814**		**1.55**
	PBE	H_e	-5.689	1.123	1.786		
	PBE-D3		-6.045	1.123	1.784		
	PBE	T	-2.962	1.835	1.179		
	PBE-D3		-3.289	1.832	1.170		
Ti	**PBE**	**H_C**	**-6.072**	**0.802**	**1.743**	**0.62**	
	PBE-D3		**-6.479**	**0.796**	**1.738**		**1.60**
	PBE	H_e	-5.524	0.901	1.716		
	PBE-D3		-5.909	0.901	1.718		
	PBE	T	-2.917	1.832	1.038		
V	**PBE**	**H_C**	**-5.348**	**0.765**	**1.508**	**-0.68**	
	PBE-D3		**-5.736**	**0.756**	**1.506**		**1.38**
	PBE	H_e	-4.681	1.073	1.459		
	PBE-D3		-5.036	1.072	1.461		
Cr	**PBE**	**H_C**	**-2.443**	**0.985**	**1.220**	**-1.56**	
	PBE-D3		**-3.046**	**0.960**	**1.236**		**0.38**
	PBE	H_e	-2.120	1.239	1.195		
	PBE-D3		-2.848	1.196	1.216		
	PBE	T	-1.665	1.893	0.827		
	PBE-D3		-2.256	1.884	0.813		
Mn	**PBE**	**H_C**	**-2.649**	**1.042**	**1.410**	**-1.21**	
	PBE-D3		**-3.024**	**1.027**	**1.411**		**0.57**
	PBE	H_e	-2.300	1.156	1.336		
	PBE-D3		-2.673	1.157	1.336		
	PBE	T	-1.490	1.926	0.858		
	PBE-D3		-1.799	1.922	0.871		
Fe	**PBE**	**H_C**	**-3.181**	**0.732**	**1.048**	**-1.69**	
	PBE-D3		**-3.461**	**0.728**	**1.056**		**0.86**
	PBE	H_e	-2.407	1.034	1.078		
	PBE-D3		-2.775	1.033	1.228		
Co	**PBE**	**H_C**	**-3.100**	**0.756**	**0.932**	**-2.17**	
	PBE-D3		**-3.394**	**0.748**	**0.925**		**0.73**
	PBE	H_e	-2.543	1.045	0.962		
	PBE-D3		-2.855	1.045	0.964		
	PBE	T	-1.520	1.796	0.684		
	PBE-D3		-1.622	1.771	0.661		
Ni	**PBE**	**H_C**	**-2.992**	**0.684**	**0.672**	**-1.88**	

	PBE-D3		**-3.331**	**0.674**	**0.674**		**0.82**
	PBE	H_e	-2.240	1.065	0.786		
	PBE-D3		-2.610	1.090	0.810		
	PBE	T	-1.754	1.763	0.605		
	PBE-D3		-2.046	1.756	0.553		
Cu	**PBE**	**H_C**	**-1.585**	**0.991**	**0.790**	**-1.90**	
	PBE-D3		**-1.938**	**0.960**	**0.795**		**0.28**
	PBE	H_e	-1.332	1.231	0.795		
	PBE-D3		-1.686	1.228	0.793		
	PBE	T	-1.109	1.828	0.618		
	PBE-D3		-1.402	1.824	0.578		
Zn	PBE	B	-0.026	3.323	0.030		
	PBE	**H_C**	**-0.030**	**3.218**	**0.042**	**-1.09**	
	PBE-D3		**-0.373**	**2.620**	**0.102**		**0.03**
	PBE	H_e	-0.027	3.228	0.036		
	PBE-D3		-0.341	2.715	0.057		
	PBE	T	-0.027	3.374	0.033		
	PBE-D3		-0.328	2.796	0.070		

Table S2. Same as Table S1 for Zr_2CO_2 (0001) surface.

Adatom		site	E_{ads} (eV)	h (Å)	ΔQ (e)	E_{diff}	E_{bar}
Sc	PBE	**H_C**	**-4.835**	**0.986**	**1.780**	**0.72**	
	PBE-D3		**-5.155**	**0.983**	**1.773**		**1.44**
	PBE	H_e	-4.194	1.084	1.696		
	PBE-D3		-4.505	1.085	1.692		
	PBE	T	-2.151	1.878	1.043		
	PBE-D3		-2.436	1.875	1.049		
Ti	**PBE**	**H_C**	**-4.696**	**0.782**	**1.620**	**-0.75**	
	PBE-D3		**-5.048**	**0.779**	**1.613**		**1.66**
	PBE	H_e	-4.001	0.866	1.661		
	PBE-D3		-4.335	0.868	1.662		
	PBE	T	-2.295	1.883	0.892		
	PBE-D3		-2.483	1.823	0.943		
V	PBE	B	-2.428	1.784	0.773		
	PBE-D3		-2.730	1.793	0.772		
	PBE	**H_C**	**-4.147**	**0.709**	**1.353**	**-1.88**	
	PBE-D3		**-4.495**	**0.714**	**1.360**		**1.50**
	PBE	H_e	-3.352	1.055	1.374		
	PBE-D3		-3.670	1.055	1.375		
	PBE	T	-2.418	1.892	0.776		
	PBE-D3		-2.708	1.891	0.726		
Cr	**PBE**	**H_C**	**-1.607**	**1.006**	**1.046**	**-2.39**	
	PBE-D3		**-2.092**	**0.972**	**1.062**		**0.54**
	PBE	T	-1.133	1.920	0.752		
	PBE-D3		-1.624	1.915	0.735		
Mn	**PBE**	**H_C**	**-1.675**	**0.949**	**1.310**	**-2.19**	
	PBE-D3		**-2.012**	**0.928**	**1.300**		**0.61**
	PBE	H_e	-1.240	1.130	1.236		

	PBE-D3		-1.580	1.133	1.234		
	PBE	T	-0.943	1.954	0.739		
	PBE-D3		-1.220	1.953	0.749		
Fe	**PBE**	**H_C**	**-2.479**	**0.695**	0.872	**-2.39**	
	PBE-D3		**-2.732**	**0.689**	0.865		**1.15**
	PBE	H_e	-1.362	1.067	1.102		
	PBE-D3		-1.675	1.028	1.103		
	PBE	T	-0.982	1.861	0.562		
	PBE-D3		-1.255	1.856	0.559		
Co	**PBE**	**H_C**	**-2.496**	**0.694**	**0.749**	**-2.77**	
	PBE-D3		**-2.763**	**0.692**	**0.744**		**0.96**
	PBE	H_e	-1.625	1.064	0.865		
	PBE-D3		-1.916	1.066	0.860		
	PBE	T	-1.112	1.842	0.508		
	PBE-D3		-1.376	1.836	0.509		
Ni	PBE	B	-1.483	1.396	0.463		
	PBE	**H_C**	**-2.589**	**0.653**	**0.509**	**-2.28**	
	PBE-D3		**-2.898**	**0.646**	**0.508**		**1.20**
	PBE	T	-1.418	1.770	0.369		
	PBE-D3		-1.690	1.767	0.389		
Cu	**PBE**	**H_C**	**-1.101**	**0.893**	**0.700**	**-2.38**	
	PBE-D3		**-1.422**	**0.873**	**0.697**		**0.59**
	PBE	T	-0.702	1.866	0.411		
	PBE-D3		-0.966	1.864	0.425		
Zn	PBE	B	-0.025	3.592	-0.030		
	PBE	**H_C**	**-0.029**	**3.462**	**-0.025**	**-1.09**	
	PBE-D3		**-0.334**	**2.711**	**0.025**		**0.02**
	PBE	H_e	-0.028	3.429	-0.025		
	PBE-D3		-0.313	2.803	0.012		
	PBE	T	-0.022	3.665	-0.028		
	PBE-D3		-0.280	2.961	0.015		

Table S3. Same as Table S1 for Hf_2CO_2 (0001) surface.

Adatom		site	E_{ads} (eV)	h (Å)	ΔQ (e)	E_{diff}	E_{bar}
Sc	PBE	**H_C**	**-3.799**	**1.005**	**1.704**	**-0.32**	
	PBE-D3		**-4.092**	**1.001**	**1.700**		**1.15**
	PBE	H_e	-3.293	1.136	1.566		
	PBE-D3		-3.557	1.136	1.564		
	PBE	T	-1.701	1.922	0.964		
	PBE-D3		-1.960	1.919	0.971		
Ti	**PBE**	**H_C**	**-3.768**	**0.883**	**1.434**	**-1.68**	
	PBE-D3		**-4.098**	**0.880**	**1.427**		**1.39**
	PBE	H_e	-2.948	0.912	1.550		
	PBE-D3		-3.238	0.912	1.551		
	PBE	T	-1.937	1.923	0.816		
	PBE-D3		-2.021	1.866	0.883		
V	**PBE**	**H_C**	**-3.343**	**0.760**	**1.235**	**-2.69**	
	PBE-D3		**-3.667**	**0.755**	**1.223**		**1.33**

	PBE	H_e	-2.634	1.113	1.330		
	PBE-D3		-2.913	1.112	1.327		
	PBE	T	-2.149	1.949	0.639		
	PBE-D3		-2.423	1.941	0.664		
Cr	**PBE**	**H_C**	**-1.120**	**1.121**	**0.990**	**-2.88**	
	PBE-D3		**-1.534**	**1.089**	**0.991**		**0.47**
	PBE	H_e	-0.714	1.425	0.963		
	PBE	T	-0.856	1.967	0.611		
	PBE-D3		-1.219	1.962	0.632		
Mn	**PBE**	**H_C**	**-1.069**	**0.932**	**1.174**	**-2.79**	
	PBE-D3		**-1.397**	**0.916**	**1.159**		**0.51**
	PBE	H_e	-0.721	1.170	1.160		
	PBE-D3		-1.023	1.170	1.146		
	PBE	T	-0.665	1.996	0.673		
	PBE-D3		-1.226	1.156	1.200		
Fe	PBE	B	-0.744	1.745	0.516		
	PBE-D3		-0.892	1.764	0.502		
	PBE	**H_C**	**-2.008**	**0.743**	**0.773**	**-2.86**	
	PBE-D3		**-2.257**	**0.739**	**0.771**		**1.14**
	PBE	H_e	-0.896	1.135	1.011		
	PBE-D3		-1.939	0.797	0.912		
	PBE	T	-0.739	1.912	0.477		
Co	**PBE**	**H_C**	**-2.064**	**0.735**	**0.639**	**-3.21**	
	PBE-D3		**-2.359**	**0.744**	**0.638**		**0.91**
	PBE	H_e	-1.246	1.121	0.835		
	PBE-D3		-1.516	1.123	0.835		
	PBE	T	-0.882	1.889	0.440		
	PBE-D3		-1.141	1.883	0.428		
Ni	**PBE**	**H_C**	**-2.245**	**0.707**	**0.441**	**-2.63**	
	PBE-D3		**-2.555**	**0.701**	**0.438**		**1.14**
	PBE	T	-1.213	1.786	0.402		
	PBE-D3		-1.481	1.778	0.419		
Cu	**PBE**	**H_C**	**-0.724**	**1.786**	**0.694**	**-2.76**	
	PBE-D3		**-1.044**	**1.778**	**0.691**		**0.42**
	PBE	H_e	-0.302	1.786	0.723		
	PBE-D3		-0.622	1.778	0.720		
	PBE	T	-0.505	1.900	0.387		
	PBE-D3		-0.767	1.895	0.365		
Zn	PBE	B	-0.032	3.601	-0.039		
	PBE	H_C	-0.031	3.445	0.005	-1.09	
	PBE-D3		**-0.332**	**2.805**	**0.021**		**0.03**
	PBE	**H_e**	**-0.039**	**3.520**	**-0.037**		
	PBE-D3		-0.311	2.838	0.040		
	PBE	T	-0.031	3.713	-0.037		
	PBE-D3		-0.281	3.038	-0.002		

Table S4. Same as Table S1 for V_2CO_2 (0001) surface.

Adatom	site	E_{ads} (eV)	h (Å)	ΔQ (e)	E_{diff}	E_{bar}

Sc	PBE	**H_C**	**-7.887**	**1.025**	**1.852**	**3.77**	
	PBE-D3		**-8.298**	**1.018**	**1.846**		**1.36**
	PBE	H_e	-7.488	1.142	1.833		
	PBE-D3		-7.874	1.141	1.830		
Ti	**PBE**	**H_C**	**-7.668**	**0.712**	**1.930**	**2.22**	
	PBE-D3		**-8.120**	**0.704**	**1.928**		**1.74**
	PBE	H_e	-7.313	0.899	1.860		
	PBE-D3		-7.725	0.899	1.857		
V	**PBE**	**H_C**	**-6.601**	**0.664**	**1.680**	**0.57**	
	PBE-D3		**-7.021**	**0.655**	**1.673**		**1.20**
	PBE	H_e	-6.387	0.974	1.598		
	PBE-D3		-6.767	0.971	1.602		
Cr	**PBE**	**H_C**	**-3.664**	**0.852**	**1.474**	**-0.34**	
	PBE-D3		**-4.307**	**0.788**	**1.465**		**1.26**
	PBE	H_e	-3.511	1.043	1.428		
	PBE-D3		-4.248	1.005	1.441		
	PBE	T	-2.511	1.882	0.938		
Mn	**PBE**	**H_C**	**-3.845**	**1.119**	**1.485**	**-0.01**	
	PBE-D3		**-4.241**	**1.107**	**1.488**		**0.55**
	PBE	H_e	-3.686	1.205	1.455		
	PBE-D3		-4.076	1.202	1.452		
Fe	**PBE**	**H_C**	**-3.813**	**0.908**	**1.373**	**-1.06**	
	PBE-D3		**-4.210**	**0.904**	**1.372**		**1.34**
	PBE	H_e	-3.703	1.020	1.359		
	PBE-D3		-4.094	1.018	1.357		
Co	PBE	H_C	-3.196	0.571	0.878		
	PBE-D3		-3.522	0.558	0.873		
	PBE	**H_e**	**-3.751**	**1.021**	**1.073**	**-1.52**	
	PBE-D3		**-4.080**	**1.020**	**1.074**		**0.63**
Ni	PBE	H_C	-3.145	1.043	1.035		
	PBE-D3		-3.481	0.999	1.026		
	PBE	**H_e**	**-3.283**	**1.063**	**0.984**	**-1.59**	
	PBE-D3		**-3.658**	**1.061**	**0.981**		**0.44**
	PBE	T	-2.278	1.793	0.736		
	PBE-D3		-2.593	1.790	0.724		
Cu	PBE	H_C	-2.244	1.204	0.884		
	PBE-D3		-2.605	1.173	0.884		
	PBE	**H_e**	**-2.264**	**1.235**	**0.877**	**-1.22**	
	PBE-D3		**-2.635**	**1.231**	**0.875**		**0.11**
	PBE	T	-1.845	1.821	0.738		
	PBE-D3		-2.160	1.818	0.723		
Zn	**PBE**	**H_C**	**-0.810**	**1.237**	**1.151**	**-0.31**	
	PBE-D3		**-1.158**	**1.209**	**1.172**		**0.29**
	PBE	H_e	-0.668	1.312	1.081		
	PBE-D3		-1.033	1.300	1.088		
	PBE	T	-0.368	2.003	0.656		
	PBE-D3		-0.678	1.980	0.639		

Table S5. Same as Table S1 for Nb_2CO_2 (0001) surface.

Adatom		site	E_{ads} (eV)	h (Å)	ΔQ (e)	E_{diff}	E_{bar}
Sc	**PBE**	**H_C**	**-6.324**	**0.951**	**1.825**	**2.20**	
	PBE-D3		**-6.836**	**0.936**	**1.815**		**1.26**
	PBE	H_e	-5.856	1.094	1.778		
	PBE-D3		-6.464	1.086	1.778		
	PBE	T	-3.155	1.860	1.166		
	PBE-D3		-3.640	1.859	1.151		
Ti	**PBE**	**H_C**	**-6.051**	**0.646**	**1.738**	**0.60**	
	PBE-D3		**-6.576**	**0.635**	**1.733**		**1.49**
	PBE	H_e	-5.628	0.857	1.751		
	PBE-D3		-6.213	0.855	1.743		
	PBE	T	-3.058	1.822	1.055		
	PBE-D3		-3.497	1.820	1.038		
V	**PBE**	**H_C**	**-5.230**	**0.669**	**1.439**	**-0.80**	
	PBE-D3		**-5.741**	**0.646**	**1.434**		**0.97**
	PBE	H_e	-4.884	1.016	1.462		
	PBE-D3		-5.465	1.007	1.469		
	PBE	T	-3.173	1.858	0.930		
	PBE-D3		-3.639	1.854	0.934		
Cr	**PBE**	**H_C**	**-2.460**	**-2.460**	**1.226**	**-1.54**	
	PBE-D3		**-2.889**	**-2.889**	**1.224**		**0.27**
	PBE	H_e	-2.264	-2.264	1.187		
	PBE-D3		-2.708	-2.708	1.187		
	PBE	T	-1.849	-1.849	0.845		
Mn	**PBE**	**H_C**	**-2.779**	**1.028**	**1.419**	**-1.08**	
	PBE-D3		**-3.286**	**1.009**	**1.409**		**0.44**
	PBE	H_e	-2.504	1.163	1.362		
	PBE-D3		-3.120	1.133	1.349		
	PBE	T	-1.722	1.931	0.904		
	PBE-D3		-2.205	1.922	0.867		
Fe	**PBE**	**H_C**	**-2.928**	**0.663**	**1.021**	**-1.94**	
	PBE-D3		**-3.298**	**0.648**	**1.013**		**0.31**
	PBE	H_e	-2.561	1.037	1.231		
	PBE-D3		-3.181	1.010	1.214		
	PBE	T	-1.538	1.868	0.771		
	PBE-D3		-2.011	1.852	0.783		
Co	**PBE**	**H_C**	**-2.986**	**0.743**	**0.905**	**-2.28**	
	PBE-D3		**-3.418**	**0.742**	**0.905**		**0.38**
	PBE	H_e	-2.748	1.019	0.966		
	PBE-D3		-3.294	0.993	0.946		
	PBE	T	-1.512	1.798	0.667		
	PBE-D3		-2.156	1.803	0.707		
Ni	**PBE**	**H_C**	**-2.826**	**0.680**	**0.623**	**-2.04**	
	PBE-D3		**-3.257**	**0.660**	**0.617**		**0.37**
	PBE	H_e	-2.387	1.051	0.831		
	PBE-D3		-2.995	1.016	0.810		
	PBE	T	-1.732	1.788	0.561		
	PBE-D3		-2.161	1.775	0.597		
Cu	**PBE**	**H_C**	**-1.635**	**1.037**	**0.773**	**-1.84**	
	PBE-D3		**-2.108**	**1.016**	**0.774**		**0.03**

	PBE	H_e	-1.517	1.215	0.791		
	PBE-D3		-2.082	1.164	0.776		
	PBE	T	-1.277	1.837	0.553		
	PBE-D3		-1.748	1.826	0.632		
Zn	PBE	B	-0.056	2.732	0.135	-1.06	
	PBE-D3		**-0.578**	**2.159**	**0.323**		**0.14**
	PBE	H_C	0.033	1.419	0.817		
	PBE-D3		-0.421	1.439	0.799		
	PBE	**H_e**	**-0.060**	**2.737**	**0.121**		
	PBE-D3		-0.557	2.255	0.236		
	PBE	T	-0.055	2.705	0.159		
	PBE-D3		-0.577	2.210	0.318		

Table S6. Same as Table S1 for Ta_2CO_2 (0001) surface.

Adatom		site	E_{ads} (eV)	h (Å)	ΔQ (e)	E_{diff}	E_{bar}
Sc	**PBE**	**H_C**	**-4.912**	**0.929**	**1.741**	**0.79**	
	PBE-D3		**-5.262**	**0.922**	**1.736**		**1.18**
	PBE	H_e	-4.524	1.116	1.729		
	PBE-D3		-4.832	1.115	1.723		
	PBE	T	-2.418	1.914	1.086		
	PBE-D3		-2.720	1.910	1.092		
Ti	**PBE**	**H_C**	**-4.674**	**0.674**	**1.566**	**-0.78**	
	PBE-D3		**-5.059**	**0.672**	**1.557**		**1.48**
	PBE	H_e	-4.098	0.938	1.658		
	PBE-D3		-4.433	0.936	1.658		
	PBE	T	-2.374	1.867	0.989		
	PBE-D3		-2.698	1.866	0.984		
V	**PBE**	**H_C**	**-4.086**	**0.763**	**1.342**	**-1.94**	
	PBE-D3		**-4.460**	**0.753**	**1.341**		**0.73**
	PBE	H_e	-3.820	1.115	1.346		
	PBE-D3		-4.149	1.115	1.348		
	PBE	T	-2.614	1.916	0.768		
	PBE-D3		-2.927	1.910	0.792		
Cr	**PBE**	**H_C**	**-1.699**	**1.213**	**1.078**	**-2.30**	
	PBE-D3		**-2.189**	**1.075**	**1.082**		**0.11**
	PBE	H_e	-1.584	1.357	1.061		
	PBE-PBE		-2.093	1.346	1.070		
	PBE	T	-1.385	1.945	0.760		
	PBE-D3		-1.803	1.938	0.785		
Mn	**PBE**	**H_C**	**-1.848**	**1.100**	**1.359**	**-2.01**	
	PBE-D3		**-2.227**	**1.070**	**1.365**		**0.36**
	PBE	H_e	-1.699	1.247	1.247		
	PBE-D3		-2.049	1.242	1.240		
	PBE	T	-1.224	1.981	0.826		
	PBE-D3		-1.529	1.975	0.840		
Fe	**PBE**	**H_C**	**-2.274**	**0.719**	**0.882**	**-2.60**	
	PBE-D3		**-2.559**	**0.714**	**0.880**		**0.56**
	PBE	H_e	-1.779	1.135	1.094		
	PBE-D3		-2.136	1.138	1.091		

	PBE	T	-1.114	1.934	0.672		
	PBE-D3		-1.381	1.948	0.706		
Co	**PBE**	**H_C**	**-2.317**	**0.778**	**0.827**	**-2.95**	
	PBE-D3		**-2.655**	**0.771**	**0.822**		**0.39**
	PBE	H_e	-2.132	1.085	0.875		
	PBE-D3		-2.449	1.087	0.875		
	PBE	T	-1.238	1.853	0.643		
	PBE-D3		-1.397	1.826	0.605		
Ni	**PBE**	**H_C**	**-2.383**	**0.722**	**0.535**	**-2.49**	
	PBE-D3		**-2.735**	**0.713**	**0.533**		**0.52**
	PBE	H_e	-1.887	1.115	0.709		
	PBE-D3		-2.258	1.116	0.699		
	PBE	T	-1.377	1.804	0.532		
	PBE-D3		-1.701	1.804	0.479		
Cu	PBE	B	-0.961	1.773	0.588		
	PBE	**H_C**	**-1.165**	**1.179**	**0.750**	**-2.32**	
	PBE-D3		**-1.518**	**1.138**	**0.749**		**0.11**
	PBE	H_e	-1.036	1.279	0.736		
	PBE-D3		-1.462	1.274	0.738		
	PBE	T	-0.904	1.870	0.572		
	PBE-D3		-1.207	1.863	0.589		
Zn	PBE	B	-0.031	3.181	0.056		
	PBE	**H_C**	**-0.034**	**3.125**	**0.062**	**-1.09**	
	PBE-D3		**-0.405**	**2.583**	**0.128**		**0.02**
	PBE	H_e	-0.033	3.132	0.060		
	PBE-D3		-0.386	2.574	0.126		
	PBE	T	-0.029	3.295	0.048		
	PBE-D3		-0.366	2.678	0.127		

Table S7. Same as Table S1 for Cr_2CO_2 (0001) surface.

Adatom		site	E_{ads} (eV)	h (Å)	ΔQ (e)	E_{diff}	E_{bar}
Sc	PBE	**E**	**-8.787**	**1.068**	**1.851**	**4.67**	
	PBE-D3		**-9.273**	**1.061**	**1.853**		**1.40**
	PBE	H_e	-8.437	1.185	1.834		
	PBE-D3		-9.008	1.177	1.839		
Ti	**PBE**	**E**	**-8.154**	**0.776**	**1.875**	**2.70**	
	PBE-D3		**-8.693**	**0.761**	**1.874**		**2.00**
	PBE	H_e	-7.801	0.940	1.854		
	PBE-D3		-8.429	0.929	1.848		
V	PBE	E	-7.011	1.052	1.570		
	PBE-D3		-7.444	1.037	1.573		
	PBE	**H_e**	**-7.177**	**1.122**	**1.572**	**1.15**	
	PBE-D3		**-7.700**	**1.114**	**1.573**		**0.98**
Cr	**PBE**	**E**	**-4.408**	**1.133**	**1.416**	**0.41**	
	PBE-D3		**-4.781**	**1.116**	**1.411**		**0.33**
	PBE	H_e	-4.349	1.204	1.372		
	PBE-PBE		-4.743	1.200	1.376		
Mn	**PBE**	**E**	**-4.781**	**1.182**	**1.501**	**0.92**	
	PBE-D3		**-5.240**	**1.175**	**1.507**		**1.53**

	PBE	H_e	-4.679	1.263	1.462		
	PBE-D3		-5.224	1.239	1.476		
Fe	**PBE**	**E**	**-4.574**	**1.039**	**1.409**	**-0.30**	
	PBE-D3		**-5.023**	**1.030**	**1.412**		**0.43**
	PBE	H_e	-4.484	1.176	1.369		
	PBE-D3		-4.995	1.146	1.364		
Co	PBE	E	-4.235	1.159	1.209		
	PBE-D3		-4.615	1.159	1.201		
	PBE	**H_e**	**-4.474**	**1.172**	**1.162**	**-0.80**	
	PBE-D3		**-4.947**	**1.153**	**1.151**		**1.30**
Ni	PBE	E	-3.869	1.218	1.096		
	PBE-D3		-4.306	1.215	1.097		
	PBE	**H_e**	**-3.946**	**1.204**	**1.066**	**-0.92**	
	PBE-D3		**-4.459**	**1.173**	**1.071**		**1.23**
Cu	PBE	E	-2.930	1.294	0.901		
	PBE-D3		-3.356	1.297	0.904		
	PBE	**H_e**	**-2.956**	**1.296**	**0.888**	**-0.52**	
	PBE-D3		**-3.429**	**1.259**	**0.900**		**0.16**
	PBE	T	-2.489	1.828	0.759		
	PBE-D3		-2.903	1.819	0.775		
Zn	**PBE**	**E**	**-1.681**	**1.250**	**1.229**	**0.56**	
	PBE-D3		**-2.096**	**1.248**	**1.231**		**0.71**
	PBE	H_e	-1.609	1.303	1.186		
	PBE-D3		-2.067	1.273	1.205		

Table S8. Same as Table S1 for Mo_2CO_2 (0001) surface.

Adatom		site	E_{ads} (eV)	h (Å)	ΔQ (e)	E_{diff}	E_{bar}
Sc	PBE	**E**	**-7.469**	**0.942**	**1.816**	**3.35**	
	PBE-D3		**-7.923**	**0.928**	**1.816**		**1.19**
	PBE	H_e	-7.066	1.128	1.778		
	PBE-D3		-7.609	0.928	1.781		
Ti	**PBE**	**E**	**-6.963**	**0.612**	**1.709**	**1.51**	
	PBE-D3		**-7.490**	**0.593**	**1.701**		**1.61**
	PBE	H_e	-6.441	0.866	1.782		
	PBE-D3		-7.048	0.855	1.798		
	PBE	T	-3.855	1.836	1.164		
	PBE-D3		-4.399	1.862	1.276		
V	**PBE**	**E**	**-5.936**	**0.612**	**1.475**	**-0.09**	
	PBE-D3		**-6.403**	**0.580**	**1.462**		**0.89**
	PBE	H_e	-5.081	0.914	1.579		
	PBE-D3		-5.573	0.867	1.608		
	PBE	T	-3.857	1.877	1.034		
	PBE-D3		-4.259	1.875	1.055		
Cr	**PBE**	**E**	**-3.404**	**1.054**	**1.308**	**-0.60**	
	PBE-D3		**-3.766**	**1.010**	**1.290**		**0.25**
	PBE	H_e	-3.261	1.219	1.250		
	PBE-PBE		-3.650	1.212	1.239		
	PBE	T	-2.596	1.912	0.889		
	PBE-D3		-2.922	1.908	0.907		

Mn	**PBE**	**E**	**-3.817**	**1.067**	**1.463**	**-0.04**	
	PBE-D3		**-4.250**	**1.054**	**1.466**		**0.45**
	PBE	H_e	-3.636	1.210	1.406		
	PBE-D3		-4.160	1.183	1.410		
	PBE	T	-2.453	1.930	1.014		
	PBE-D3		-2.879	1.922	1.008		
Fe	**PBE**	**E**	**-3.681**	**0.898**	**1.308**	**-1.19**	
	PBE-D3		**-4.112**	**0.876**	**1.305**		**0.40**
	PBE	H_e	-3.445	1.102	1.275		
	PBE-D3		-3.976	1.073	1.284		
Co	PBE	E	-3.395	0.992	1.068		
	PBE-D3		-3.766	0.971	1.070		
	PBE	**H_e**	**-3.573**	**1.112**	**1.052**	**-1.70**	
	PBE-D3		**-4.032**	**1.088**	**1.056**		**0.47**
	PBE	T	-2.359	1.827	0.904		
	PBE-D3		-2.624	1.829	0.854		
Ni	PBE	E	-3.064	1.087	0.992		
	PBE-D3		-3.475	1.079	0.994		
	PBE	**H_e**	**-3.081**	**1.128**	**0.941**	**-1.79**	
	PBE-D3		**-3.591**	**1.095**	**0.948**		**0.34**
	PBE	T	-2.360	1.808	0.795		
	PBE-D3		-2.786	1.804	0.739		
Cu	**PBE**	**E**	**-2.314**	**1.128**	**0.831**		
	PBE-D3		-2.725	**1.132**	0.829		
	PBE	H_e	-2.274	1.239	0.812	-1.21	
	PBE-D3		**-2.752**	**1.200**	**0.821**		**0.10**
	PBE	T	-1.973	1.834	0.730		
	PBE-D3		-2.390	1.825	0.725		
Zn	**PBE**	**E**	**-0.832**	**1.229**	**1.110**	**-0.29**	
	PBE-D3		**-1.233**	**1.239**	**1.103**		**0.43**
	PBE	H_e	-0.695	1.358	1.004		
	PBE-D3		-1.126	1.304	1.043		
	PBE	T	-0.484	2.024	0.663		
	PBE-D3		-0.931	2.185	0.546		

Table S9. Same as Table S1 for W_2CO_2 (0001) surface.

Adatom		site	E_{ads} (eV)	h (Å)	ΔQ (e)	E_{diff}	E_{bar}
Sc	PBE	**E**	**-5.759**	**1.094**	**1.729**	**1.64**	
	PBE-D3		**-6.119**	**1.087**	**1.731**		**0.97**
	PBE	H_e	-5.475	1.229	1.703		
	PBE-D3		-5.798	1.227	1.700		
	PBE	T	-3.550	1.941	1.272		
	PBE-D3		-3.789	1.935	1.222		
Ti	**PBE**	**E**	**-5.099**	**1.044**	**1.594**	**-0.35**	
	PBE-D3		**-5.489**	**1.026**	**1.596**		**0.91**
	PBE	H_e	-5.050	1.304	1.544		
	PBE-D3		-5.400	1.303	1.548		
	PBE	T	-3.308	1.909	1.132		
	PBE-D3		-3.622	1.905	1.123		

V	PBE	E	-4.926	1.228	1.440		
	PBE-D3		-5.281	1.219	1.444		
	PBE	**H_e**	**-4.964**	**1.252**	**1.422**	**-1.07**	
	PBE-D3		**-5.298**	**1.251**	**1.422**		**0.56**
	PBE	T	-3.565	1.964	1.063		
	PBE-D3		-3.842	1.937	0.990		
Cr	PBE	E	-2.678	1.402	1.192		
	PBE-D3		-3.125	1.380	1.199		
	PBE	**H_e**	**-2.686**	**1.429**	**1.174**	**-1.31**	
	PBE-PBE		**-3.170**	**1.422**	**1.172**		**0.12**
	PBE	T	-2.323	1.964	0.870		
	PBE-D3		-2.747	1.958	0.888		
Mn	**PBE**	**E**	**-2.883**	**1.223**	**1.478**	**-0.98**	
	PBE-D3		**-3.247**	**1.200**	**1.488**		**0.35**
	PBE	H_e	-2.835	1.324	1.403		
	PBE-D3		-3.185	1.323	1.403		
Fe	PBE	E	-2.660	1.223	1.255		
	PBE-D3		-3.018	1.242	1.259		
	PBE	**H_e**	**-2.710**	**1.299**	**1.223**	**-2.16**	
	PBE-D3		**-3.087**	**1.297**	**1.220**		**0.30**
	PBE	T	-1.781	1.922	0.860		
Co	PBE	E	-2.763	1.280	1.064		
	PBE-D3		-3.073	1.264	1.066		
	PBE	**H_e**	**-2.904**	**1.239**	**1.028**	**-2.37**	
	PBE-D3		**-3.223**	**1.238**	**1.023**		**0.32**
	PBE	T	-2.047	1.867	0.853		
	PBE-D3		-2.360	1.866	0.816		
Ni	PBE	E	-2.509	1.297	0.974		
	PBE-D3		-2.858	1.281	0.976		
	PBE	**H_e**	**-2.603**	**1.253**	**0.950**	**-2.27**	
	PBE-D3		**-2.973**	**1.251**	**0.948**		**0.17**
	PBE	T	-2.079	1.851	0.780		
	PBE-D3		-2.388	1.851	0.780		
Cu	PBE	E	-1.919	1.405	0.823		
	PBE-D3		-2.269	1.379	0.798		
	PBE	**H_e**	**-1.950**	**1.370**	**0.827**	**-1.53**	
	PBE-D3		**-2.324**	**1.368**	**0.829**		**0.09**
	PBE	T	-1.711	1.859	0.761		
	PBE-D3		-2.031	1.856	0.734		
Zn	**PBE**	**E**	**-0.325**	**1.648**	**0.802**		
	PBE-D3		-0.650	1.630	0.802		
	PBE	H_e	-0.305	1.663	0.789	-0.81	
	PBE-D3		**-0.666**	**1.646**	**0.791**		**0.09**
	PBE	T	-0.217	2.148	0.581		
	PBE-D3		-0.651	2.225	0.532		

Table S10. The linear regression y= a + bx parameters and R^2 factor of trends reported in Fig. 6.

M of MXene	Parameters		factor
	a	b	R^2
Ti	-1.33	1.26	0.42
Zr	-0.19	0.83	0.38
Hf	0.07	0.62	0.37
V	-1.68	1.47	0.54
Nb	-1.13	1.16	0.51
Ta	-1.05	0.92	0.52
Cr	-1.39	1.50	0.74
Mo	-1.88	1.39	0.70
W	-0.92	0.99	0.64

Tabla S11. Electronic configurations of the transition metal atoms.

Element	Electronic configuration
Sc	[Ar] $4s^2$ $3d^1$
Ti	[Ar] $4s^2$ $3d^2$
V	[Ar] $4s^2$ $3d^3$
Cr	[Ar] $4s^1$ $3d^5$
Mn	[Ar] $4s^2$ $3d^5$
Fe	[Ar] $4s^2$ $3d^6$
Co	[Ar] $4s^2$ $3d^7$
Ni	[Ar] $4s^2$ $3d^8$
Cu	[Ar] $4s^1$ $3d^{10}$
Zn	[Ar] $4s^2$ $3d^{10}$
Zr	[Kr] $5s^2$ $4d^2$
Nb	[Kr] $5s^1$ $4d^4$
Mo	[Kr] $5s^1$ $4d^5$
Hf	[Xe] $6s^2$ $5d^2$
Ta	[Xe] $6s^2$ $5d^3$
W	[Xe] $6s^2$ $5d^4$

Tabla S12. Electronegativities of the transition metal atoms.[a]

Ti	V	Cr
(1.54)	(1.63)	(1.66)
Zr	Nb	Mo
(1.33)	(1.60)	(2.16)
Hf	Ta	W
(1.30)	(1.50)	(2.36)

[a] John Emsley, *The Elements*, 3rd Edition. Oxford:Clarendon Press, 1998.