Supplementary Material for:

Methane on a Stepped Surface: Dynamical Insights on the Dissociation of CHD$_3$ on Pt(111) and Pt(211)

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The Tables contain the details about the data and the distributions reported in the main paper. For each dataset are reported: the Figure title, the Figure number in the main paper, the Panel of the Figure, the dataset name, the average ± the standard error (σ_M), the standard deviation of the dataset (σ), the bin size and the broadening parameter (σ_G) used for the Gaussian binning of the data and the data unit.

Steering

Fig.	Panel	Set	Average ± σ_M	σ	Bin size	σ_G	unit
5	A	Pt(111) Reactive	0.0684 ± 0.002	0.0483	0.005	0.01	Å
5	A	Pt(111) Scattered	0.0522 ± 0.0004	0.0298	0.005	0.01	Å
5	B	Pt(211) Reactive – edge	0.0882 ± 0.005	0.0677	0.005	0.01	Å
5	B	Pt(211) Reactive – bot&low	0.1412 ± 0.01	0.0797	0.005	0.01	Å
5	B	Pt(211) Scattered – step	0.1856 ± 0.002	0.1043	0.005	0.01	Å
5	B	Pt(211) Scattered - terrace	0.1169 ± 0.001	0.0654	0.005	0.01	Å
5	C	Pt(211) Trapped – all	0.2233 ± 0.02	0.1145	0.005	0.01	Å
5	C	Pt(211) Trapped – step	0.2494 ± 0.02	0.1190	0.005	0.01	Å
5	C	Pt(211) Trapped – terrace	0.1507 ± 0.02	0.0589	0.005	0.01	Å

Distance travelled and $\langle v_{xy} \rangle^{trap}$

Fig.	Panel	Set	Average ± σ_M	σ	Bin size	σ_G	unit
6	A	Pt(111) Reactive	0.0730 ± 0.002	0.0465	0.05	0.05	Å
6	A	Pt(111) Scattered	0.7678 ± 0.005	0.4122	0.05	0.05	Å
6	B	Pt(211) Reactive	0.1080 ± 0.004	0.0716	0.05	0.05	Å
6	B	Pt(211) Scattered b = 0	2.8168 ± 0.02	1.8	0.05	0.05	Å
6	B	Pt(211) Scattered b > 0	16.9394 ± 1.3	7.9	0.05	0.05	Å
6	C	Pt(211) XY	25.4 ± 1.6	9.3	0.1	0.8	Å
6	C	Pt(211) X	23.2 ± 1.8	10.5	0.1	0.8	Å
6	C	Pt(211) Y	7.3 ± 0.8	4.4	0.1	0.8	Å
6	D	Pt(211) V_{xy} all	0.0138 ± 0.0009	0.005	0.0005	0.001	Å/fs
6	D	Pt(211) V_{xy} step	0.0149 ± 0.001	0.005	0.0005	0.001	Å/fs
6	D	Pt(211) V_{xy} terrace	0.0106 ± 0.001	0.004	0.0005	0.001	Å/fs

K_{xy}

Fig.	Panel	Set	Average ± σ_M	σ	Bin size	σ_G	unit
7	A	Pt(211) Step scattered	18.5 ± 0.3	13.9	0.5	0.8	kJ/mol
7	A	Pt(211) Terrace scattered	11.2 ± 0.2	10.2	0.5	0.8	kJ/mol
7	B	Pt(211) Step trapped	14.1 ± 2.8	14.1	0.5	0.8	kJ/mol
7	B	Pt(211) Terrace trapped	11.5 ± 2.7	8.0	0.5	0.8	kJ/mol

$\langle v_x \rangle^{trap}$

Fig.	Panel	Set	Average ± σ_M	σ	Bin size	σ_G	unit
10	-	Pt(211) All trapped	0.0081 ± 0.002	0.0113	0.0005	0.001	Å/fs
10	-	Pt(211) Step trapped	0.0137 ± 0.001	0.0057	0.0005	0.001	Å/fs
10	-	Pt(211) Terrace trapped	-0.0075 ± 0.002	0.0074	0.0005	0.001	Å/fs

Energy Transfer

Fig.	Panel	Set	Average ± σ_M	σ	Bin size	σ_G	unit
11	A	Pt(111) Scattered	15.53 ± 0.15	12.4	1.0	2.0	kJ/mol
11	A	Pt(211) Scattered	13.90 ± 0.18	13.1	1.0	2.0	kJ/mol
11	A	Pt(211) Trapped	23.17 ± 1.91	11.2	1.0	2.0	kJ/mol

Distance from top

Fig.	Panel	Set	Average ± σ_M	σ	Bin size	σ_G	unit
12	A	Pt(111) Reactive t = 0	0.65 ± 0.02	0.35	0.05	0.05	Å
12	A	Pt(111) Reactive t = t_{diss}	0.65 ± 0.02	0.34	0.05	0.05	Å
12	A	Pt(111) Scattered t = 0	1.02 ± 0.004	0.35	0.05	0.05	Å
12	B	Pt(211) Reactive t = 0	0.78 ± 0.02	0.34	0.05	0.05	Å
12	B	Pt(211) Reactive t = t_{diss}	0.80 ± 0.02	0.35	0.05	0.05	Å
12	B	Pt(211) Scattered t = 0	0.99 ± 0.004	0.36	0.05	0.05	Å
12	B	Pt(211) Trapped t = 0	1.02 ± 0.08	0.44	0.05	0.05	Å

β

Fig.	Panel	Set	Average ± σ_M	σ	Bin size	σ_G	unit
13	A	Pt(111) Reactive t = 0	134 ± 0.9	20	1	2	°
13	A	Pt(111) Reactive t = t_{diss}	150 ± 0.6	12	1	2	°
13	B	Pt(211) Reactive t = 0	123 ± 1.4	22	1	2	°
13	B	Pt(211) Reactive t = t_{diss}	141 ± 1.1	17	1	2	°

θ

Fig.	Panel	Set	Average ± σ_M	σ	Bin size	σ_G	unit
14	A	Pt(111) Reactive t = 0	134 ± 0.9	19	1	2	°
14	A	Pt(111) Reactive t = t_{diss}	124 ± 0.5	10	1	2	°
14	B	Pt(211) Reactive t = 0	124 ± 1.4	21	1	2	°
14	B	Pt(211) Reactive t = t_{diss}	117 ± 1.0	15	1	2	°

γ

Fig.	Panel	Set	Average ± σ_M	σ	Bin size	σ_G	unit
15	-	Pt(111) Reactive t = 0	13.4 ± 0.3	7	1	2	°
15	-	Pt(111) Reactive t = t_{diss}	33.8 ± 0.6	13	1	2	°
15	-	Pt(211) Reactive t = 0	12.9 ± 0.4	7	1	2	°
15	-	Pt(211) Reactive t = t_{diss}	31.9 ± 0.8	12	1	2	°

β, θ and γ vs. $\langle E_i \rangle$ – linear regressions parameters				
Fig.	Panel	Set	Slope [° * mol/kJ]	Intercept [°]
16	A	Pt(111) β	0.00	150
16	A	Pt(211) β	0.01	141
16	B	Pt(111) θ	-0.14	137
16	B	Pt(211) θ	-0.22	136
16	C	Pt(111) γ	0.12	22
16	C	Pt(211) γ	0.13	21