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Supplementary Material: H2 Thermal Desorption Spectra on Pt(111), a Density Functional Theory and Kinetic Monte Carlo Simulation Study

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Tables

Table S1 Frequencies of H(a) on Pt(111) and H_2.

	H-fcc / cm^{-1}	H-hcp / cm^{-1}	H-top / cm^{-1}	H_2-fcc/ cm^{-1}
1	1021.34	1048.26	2194	4330.35
2	612.96	534.08	467	296.41
3	561.93	481	419	158.89
4				134.14
5				55.85
6				112.56*

Table S2 Frequencies of 2H-fcc, transition state and H_2.

	f_{IS} / cm^{-1}	f_{TS} / cm^{-1}	f_{FS} / cm^{-1}
1	1047.60	2173.37	4330.35
2	1021.78	1592.86	296.41
3	653.97	466.69	158.89
4	609.50	295.45	134.14
5	586.16	137.14	55.85
6	567.58	377.01*	112.56*

The asterisk * indicates the imaginary frequency.

Table S3 Frequencies of H-fcc, transition state and H-hcp.

	f_{IS} / cm^{-1}	f_{TS} / cm^{-1}	f_{FS} / cm^{-1}
1	1021.34	1214.71	1048.26
2	612.96	813.54	534.08
3	561.93	257.91*	480.98

Table S4 The pre-exponential factors of H_2 desorption and H(a) diffusion.

Process	$\nu_{forward}$	$\nu_{reverse}$
H_2 desorption	6.80×10^{13}	1.19×10^{11}
H(a) diffusion	1.07×10^{13}	8.17×10^{12}

Table S5 E_{ads}(eV) of the typical configurations of H(a) and H_2; E_a of H(a) diffusion and H_2 desorption on Pt(111) by DFT and DFT-D methods.

	RPBE	PBE	PBE-D
H-fcc	-0.384	-0.532	-0.532
2H-fcc	-0.734	-1.040	-1.042
3H-fcc	-1.062	-1.529	-1.535
H_2-fcc	-0.004	-0.018	-0.018
H(a) diffusion	0.074	0.073	0.074
H_2 desorption	0.923	1.160	1.161

Figure

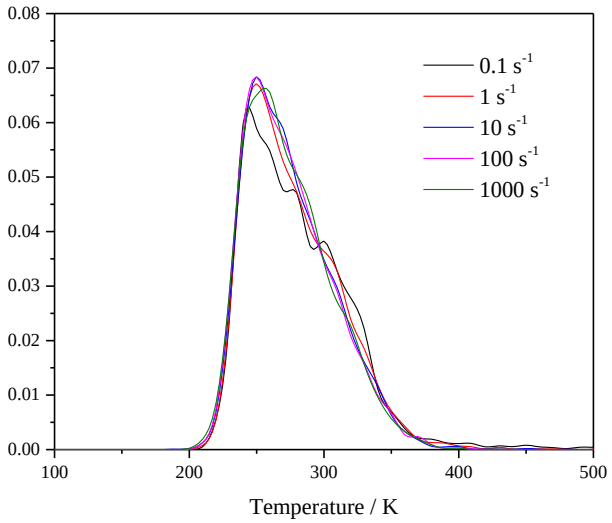

Figure S1. Effects of the diffusion rate constant on the H_2 TDS spectra by kMC simulation.