Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Accessing the C-C Transition State Energy on Transition Metals

Hassan Aljama[1,2] and Frank Abild-Pedersen[1,2]

[1]Department of Chemical Engineering, Stanford University, 443 Via Ortega, Stanford, CA 94305 United States
[2]SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, California, 94025 United States

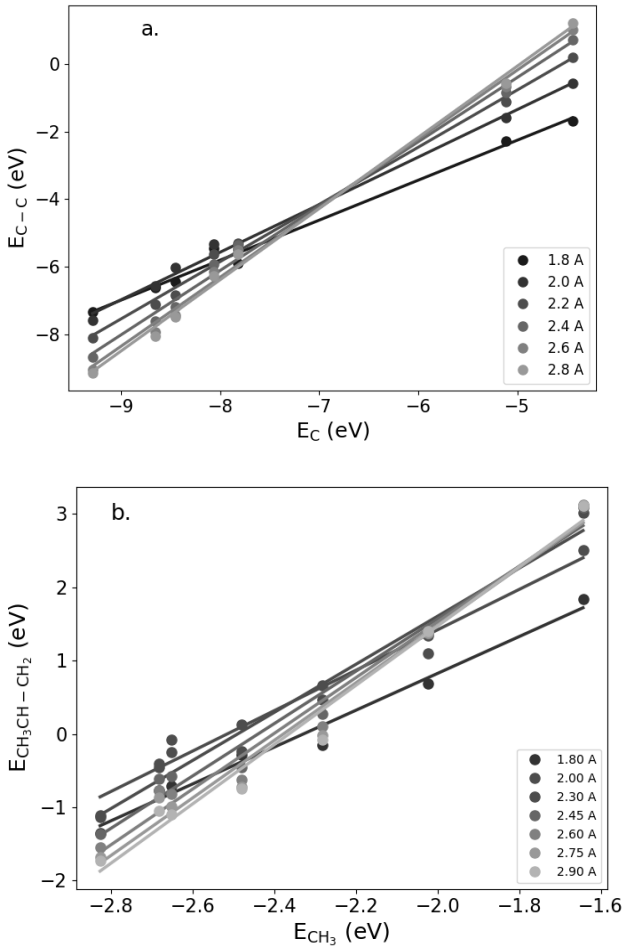

Figure S1: The binding energy of a. diatomic carbon (C-C) and b. propylene (CH_3CH-CH_2) at different C-C bond lengths. At C-C bond distance of 1.8-2.8 Å, all transition metals follow the same scaling line

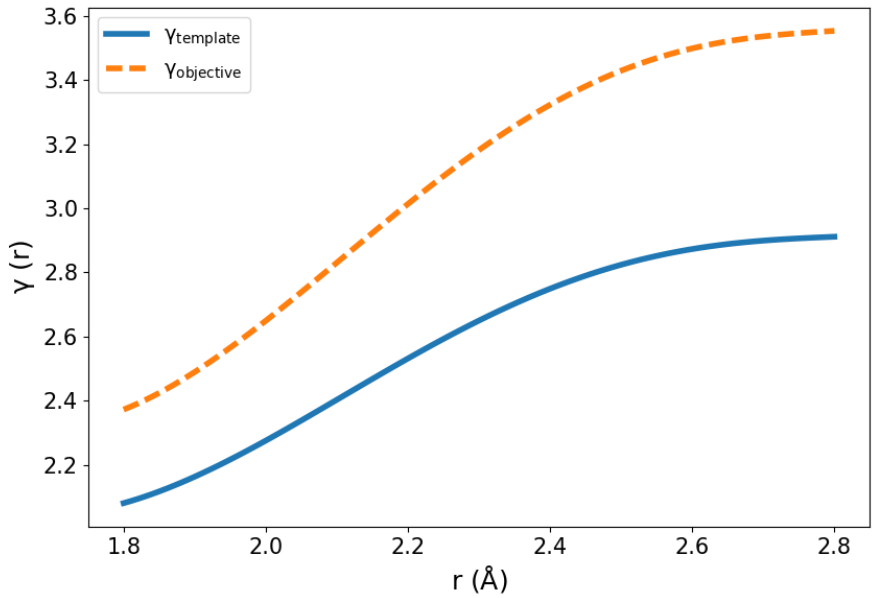

Figure S2: Example illustration of the hetero-transfer approach (adapted from [1]). The objective function ($\gamma_{objective}$) is rescaled from the template function ($\gamma_{template}$) using the initial and final values: $\gamma_{objective}$(r) = $\gamma_{objective}$(1.8) + ([($\gamma_{objective}$)(2.8) - ($\gamma_{objective}$)(1.8)]x[($\gamma_{template}$)(r) - ($\gamma_{template}$)(1.8)])/(($\gamma_{template}$)(2.8) - ($\gamma_{template}$)(1.8)). The initial and final states are taken at 1.8 and 2.8 Å, respectively, in this case

Table S1: Range of the transition state C-C bond distances (Å) for different hydrocarbons on noble and reactive metals based on CI-neb calculations

Transition State	Facet	Reactive Metals	Noble Metals
C-C	211	1.8-2.4	2.4-2.9
CC-C	211	1.5-1.9	
CH-CH	211	2.4	2-2.2
CH_2-CH_2	211	2-2.2	
CH_2-$CHCH_3$	211	2-2.2	2.5-3.0
C-C	111	1.95-2.4	2.1-2.7
CH-CH	111	1.9-2.4	2.5-2.7
CH_2-CH_2	111	2	3.2

Table S2: Binding energies (eV) of different hydrocarbons on transition metal surfaces

Metal	Facet	C	CH_2	CH_3	CH
Ru	211	-8.69	-4.91	-2.68	-7.07
Pt	211	-7.70	-5.01	-2.65	-6.34
Ag	211	-4.46	-2.73	-1.64	-3.77
Re	211	-9.38	-5.39	-2.83	-7.40
Au	211	-5.14	-3.44	-1.96	-4.28
Pd	211	-8.20	-4.55	-2.28	-6.32
Rh	211	-8.46	-4.72	-2.48	-6.55
Cu	211	-6.12	-3.60	-2.02	-5.16
Ru	111		-4.76		
Pt	111		-4.43		
Ag	111		-2.38		
Re	111		-4.86		
Au	111		-2.92		
Pd	111		-4.22		
Rh	111		-4.40		
Cu	111		-3.14		

Table S3: Transition state energies (eV) for C-C bond dissociation on different hydrocarbons based on CI-neb

Metal	Facet	CH_2-$CHCH_3$	CH_3-CCH_2	C-C	CH-C	CH-CH	CH_2-CH_2	C-CCH_3
Ru	211	-0.29	-2.64	-6.45	-4.61	-1.39	-0.22	
Pt	211					-0.11		
Ag	211	3.09		1.28				
Re	211	-1.04		-7.61		-2.58	-0.95	
Au	211			-0.51				
Pd	211	0.99		-4.92		-0.02	1.15	
Rh	211			-5.98	-4.12	-0.62	0.09	
Cu	211	1.36	0.22		-0.99	1.41		
Ru	111					-1.79	0.16	-4.51
Pt	111			-4.29				
Ag	111			1.23		4.19		2.46
Re	111			-6.34		-2.18	-0.05	
Au	111							
Pd	111			-4.51		-0.17	1.22	
Rh	111			-5.36		-1.25		
Cu	111			-1.57		1.67	2.52	-0.21

Table S4: Comparison between Model Results and Literature Values

Transition State	Surface	Model Preiction (eV)	Literature (eV)	Reference
CH_2-CH_2	Pt(111)	2.21	2.06	[2]
CH_2-CH_2	Pd(111)	1.93	1.68	[3]
CH-CH	Pd(111)	1.57	1.47	[3]
C-C	Pd(111)	1.39	1.25	[4]
C-C	Rh(111)	1.25	1.17	[4]

Table S5: Tabulated γ(r) and ξ(r) values. Note that the descriptor for CH-CH (211) is CH* on (211), C-C (111) is C* on (111), and CH_3CH-CH_2 (211) is CH_2* on (211) as discussed in the text and Figure 6

	CH-CH (211)		C-C (111)		CH_3CH-CH_2 (211)	
r (A)	γ(r)	ξ(r)	γ(r)	ξ(r)	γ(r)	ξ(r)
1.8	2.11	7.89	1.18	3.64	2.73	6.44
2	2.22	8.89	1.4	5.67	2.88	7.29
2.15					3.30	8.44
2.2	2.55	10.17	1.69	7.67		
2.3					3.65	9.19
2.4	2.76	10.76	1.9	9.1		
2.45					3.84	9.46
2.6	2.87	11.04	2.04	10	4.00	9.68
2.75					4.07	9.72
2.8	2.91	11.09	2.1	10.45		

References

(1) L. Yu, L. Vilella and F. Abild-Pedersen, *Communications Chemistry*, 2018, **1**, 2.

(2) E. Shustorovich, *Catalysis Letters*, 1990, **7**, 107–118.

(3) Z.-X. Chen, H. A. Aleksandrov, D. Basaran and N. Rösch, *The Journal of Physical Chemistry C*, 2010, **114**, 17683–17692.

(4) D. Basaran, H. A. Aleksandrov, Z.-X. Chen, Z.-J. Zhao and N. Rösch, *Journal of Molecular Catalysis A: Chemical*, 2011, **344**, 37–46.