

Electronic Supplementary Information

**Bond-Energy Decoupling: Principle and Application to
Heterogeneous Catalysis**

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Supplementary figures

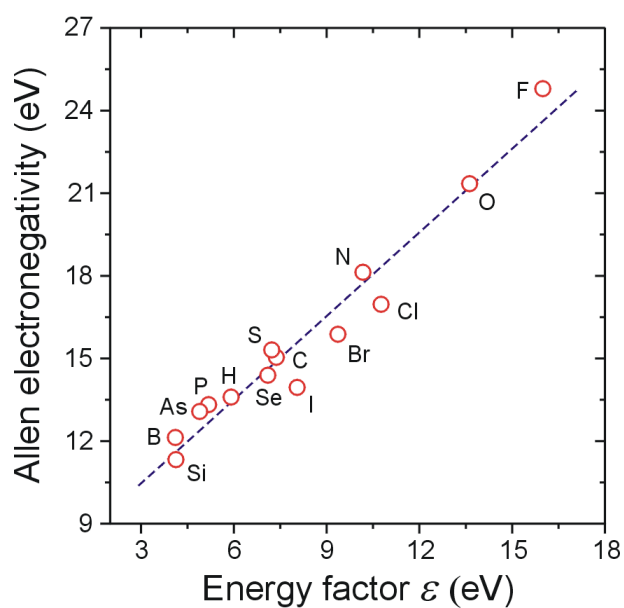


Figure S1 Correlation between the energy factor (ϵ) and the Allen electronegativity which represents the average energy of valence electrons.

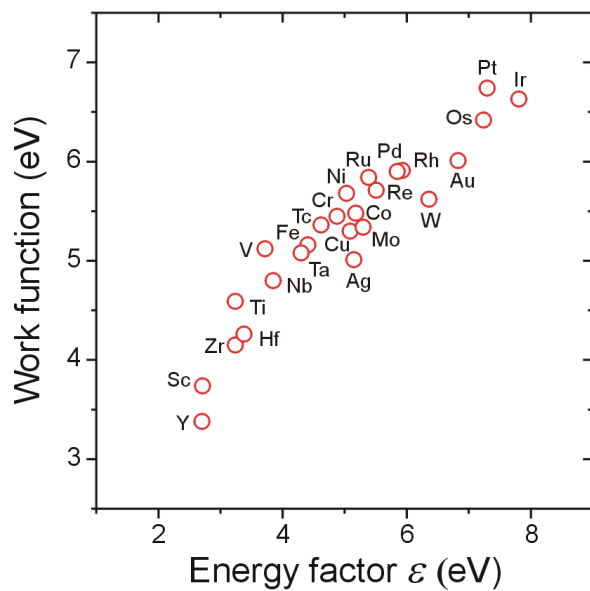


Figure S2 Correlation between the energy factor (ϵ) and the work function of 25 transition metal surfaces here studied (Table 1).

Supplementary tables

Table S1 The bond energy of 175 single bonds collected from the literature.¹¹⁻¹³

bond	bond energy (eV)	bond	bond energy (eV)
H-H	4.478	<i>t</i> C ₄ H ₉ - <i>t</i> C ₄ H ₉	3.305
F-F	1.605	C ₆ H ₅ -C ₆ H ₅	4.921
Cl-Cl	2.473	C ₆ H ₅ CH ₂ -CH ₂ C ₆ H ₅	2.788
Br-Br	1.970	C ₆ F ₅ -C ₆ F ₅	5.022
I-I	1.539	S-S	2.168
O-O	1.401	HS-SH	2.767
HO-OH	2.144	CH ₃ S-SCH ₃	2.788
CH ₃ O-OCH ₃	1.696	HCC-CCH	6.908
N-N	1.626	CH ₂ CH-CHCH ₂	5.030
NH ₂ -NH ₂	2.832	B-B	3.048
C-C	3.565	Si-Si	1.791
CH ₃ -CH ₃	3.872	SiH ₃ -SiH ₃	3.288
CH ₃ CO-COCH ₃	3.144	P-P	2.186
C ₂ H ₅ -C ₂ H ₅	3.725	As-As	1.353
<i>i</i> C ₃ H ₇ - <i>i</i> C ₃ H ₇	3.625	Se-Se	1.869
F-N	2.759	F-CH ₃	4.732
H-N	4.012	HO-SH	3.002
I-COCH ₃	2.273	HO-C ₂ H ₅	4.017
I-OH	2.174	F-CHCH ₂	5.327
NH ₂ -COCH ₃	4.259	F-Cl	2.665
F-I	2.776	H-COCH ₃	3.838
Br-OH	2.134	F-Si	5.569
OCH ₃ -COCH ₃	4.360	CH ₃ O-C ₂ H ₅	3.643
I-B	2.758	F-C ₂ H ₅	4.599
F-COCH ₃	5.265	Br-As	2.412
Br-Se	2.303	Cl-OH	2.382
F-O	1.879	Br-O	1.962
HO-COCH ₃	4.723	NH ₂ -C ₆ H ₅	4.411
H-CH ₃	4.515	F-C ₆ F ₅	4.989
H- <i>t</i> C ₄ H ₉	4.112	I-As	1.766
H-F	5.866	NH ₂ -CH ₂ C ₆ H ₅	3.141
Cl-COCH ₃	3.631	F-S	3.657
Br-COCH ₃	2.988	COCH ₃ - <i>i</i> C ₃ H ₇	3.488
HO-C ₆ F ₅	4.594	H-P	3.275
Cl-CCH	4.477	Br-CH ₃	3.010
H-OCH ₃	4.524	Cl- <i>t</i> C ₄ H ₉	3.609
H-CCH	5.743	Br-P	2.798
F- <i>t</i> C ₄ H ₉	5.101	CH ₃ -B	3.834
F-OH	2.191	CH ₃ CO-CH ₂ C ₆ H ₅	3.068

Br-C ₆ H ₅	3.449	CH ₃ O-C ₆ H ₅	4.303
Cl-SiH ₃	4.709	HO-CH ₃	3.952
C ₆ H ₅ -CH ₂ C ₆ H ₅	3.939	Cl-C	3.366
CH ₃ CO-C ₆ H ₅	4.177	I-C	2.451
CH ₃ -SiH ₃	3.849	H-S	3.479
F-Br	2.864	F-B	6.647
H-CH ₂ C ₆ H ₅	3.854	CH ₃ O- <i>i</i> C ₃ H ₇	3.700
F-NH ₂	2.932	Cl-CH ₂ C ₆ H ₅	3.070
CH ₃ - <i>t</i> C ₄ H ₉	3.730	H-NH ₂	4.627
CH ₃ CO- <i>t</i> C ₄ H ₉	3.375	HO-CH ₂ C ₆ H ₅	3.425
CH ₃ O- <i>t</i> C ₄ H ₉	3.622	CH ₃ - <i>i</i> C ₃ H ₇	3.786
H-C ₆ F ₅	5.014	Br-S	2.161
H-SCH ₃	3.752	Cl-I	2.152
Br-CHCH ₂	3.468	Cl-As	2.950
H- <i>i</i> C ₃ H ₇	4.217	Br-B	3.735
H-Se	3.319	Cl-O	2.065
<i>t</i> C ₄ H ₉ -SH	3.084	Cl-Br	2.235
Br-CH ₂ C ₆ H ₅	2.442	CH ₃ -CH ₂ C ₆ H ₅	3.331
H-C ₂ H ₅	4.320	CH ₃ CO-C ₂ H ₅	3.562
Cl-B	4.590	H-B	3.797
OH-C ₆ H ₅	4.767	HO- <i>i</i> C ₃ H ₇	4.086
Cl-C ₆ F ₅	3.935	HO- <i>t</i> C ₄ H ₉	4.090
H-I	3.053	F-CCH	5.365
NH ₂ - <i>i</i> C ₃ H ₇	3.669	F-P	5.107
F- <i>i</i> C ₃ H ₇	4.976	Cl- <i>i</i> C ₃ H ₇	3.631
F-C ₆ H ₅ CH ₂	4.240	Cl-CH ₃	3.592
H-C ₆ H ₅	4.856	Cl-N	2.031
Cl-Se	2.619	CH ₃ -COCH ₃	3.609
Cl-Si	3.678	H-Cl	4.433
H-C	4.246	Br-I	1.818
I-Si	2.169	CH ₃ O-CH ₃	3.609
F-SiH ₃	6.574	H-SH	3.913
NH ₂ -CH ₃	3.653	Br- <i>i</i> C ₃ H ₇	3.063
CH ₃ -C ₆ F ₅	4.515	Br- <i>t</i> C ₄ H ₉	2.998
Cl-C ₆ H ₅	4.104	I-SiH ₃	3.061
Cl-C ₂ H ₅	3.613	CH ₃ -C ₆ H ₅	4.385
H-O	4.758	H-Br	3.757
NH ₂ -C ₂ H ₅	3.613	H-OH	5.114
Br-C	2.820	H-Si	3.015
H-CHCH ₂	4.773	OH-OCH ₃	1.922
Cl-CHCH ₂	4.071	F-As	4.788
F-Se	3.553	Br-C ₂ H ₅	2.998
Br-CCH	4.217	I-P	2.191
Br-SiH ₃	3.859	HS-SCH ₃	2.781

Cl-S	2.551	CH ₃ -C ₂ H ₅	3.800
HO-SCH ₃	3.111	F-C ₆ H ₅	5.408
F-C	4.533	H-SiH ₃	3.939
Br-Si	2.959	Cl-P	3.392
NH ₂ - <i>t</i> C ₄ H ₉	3.648		

Table S2 The energy factor (ε) and the phase factor (θ) of 30 reactants involved in Figure 1a.

reactant	ε (eV)	θ (rad)	reactant	ε (eV)	θ (rad)
-H	5.798	0.455	- <i>t</i> C ₄ H ₉	6.363	0.369
-F	16.036	0.159	-C ₆ H ₅	7.057	0.431
-Cl	10.768	0.242	-CH ₂ C ₆ H ₅	7.169	0.317
-Br	9.373	0.231	-C ₆ F ₅	7.774	0.414
-I	7.908	0.222	-S	7.495	0.272
-O	13.038	0.165	-SH	8.288	0.293
-OH	13.089	0.204	-SCH ₃	7.944	0.301
-OCH ₃	12.639	0.184	-C \equiv CH	8.979	0.454
-N	9.752	0.206	-CH=CH ₂	7.377	0.425
-NH ₂	10.687	0.260	-B	4.255	0.437
-C	7.383	0.355	-Si	4.336	0.327
-CH ₃	7.324	0.372	-SiH ₃	4.368	0.449
-COCH ₃	5.491	0.388	-P	5.186	0.330
-C ₂ H ₅	7.211	0.368	-As	4.897	0.266
- <i>i</i> C ₃ H ₇	6.743	0.375	-Se	7.119	0.259

Table S3 The bond energies of 80 covalent bonds predicted using Eq. 1 and from *ab initio* calculations (Data are plotted in Figure 1b).

bond	predicted (eV)	theoretical (eV)	bond	predicted (eV)	theoretical (eV)
CH ₂ CH- <i>i</i> C ₃ H ₇	4.342	4.341	Se-OH	3.000	2.973
CH ₃ S-COCH ₃	3.280	3.276	S-COCH ₃	2.924	2.892
CH ₂ CH-COCH ₃	4.173	4.164	Se-NH ₂	2.661	2.701
CH ₂ CH-CCH	6.006	6.019	CH ₃ S- <i>t</i> C ₄ H ₉	3.150	3.195
SH-N	2.302	2.289	NH ₂ -OCH ₃	2.427	2.380
HS-O	2.703	2.716	HCC-SCH ₃	4.707	4.659
CH ₃ CO-O	4.182	4.167	<i>i</i> C ₃ H ₇ -OCH ₃	3.830	3.775
CH ₃ S-O	2.851	2.833	CH ₃ O-Cl	2.146	2.201
SH-Br	2.419	2.441	B-CHCH ₂	4.326	4.383
CH ₃ S-N	2.368	2.341	CH ₂ CH-NH ₂	4.420	4.362
HS-OH	2.973	3.104	B-OCH ₃	5.208	5.007

SiH ₃ -SCH ₃	3.594	3.726	CH ₃ S-NH ₂	2.864	3.067
CH ₃ S-OH	3.082	3.219	S-OH	3.227	3.016
SH-Cl	2.703	2.842	B-SH	3.944	3.732
CH ₂ CH-OCH ₃	4.367	4.226	CH ₃ S-S	2.727	2.510
HCC-COCH ₃	5.014	5.158	P-SH	2.650	2.870
Se-SH	2.517	2.367	CH ₃ -N	3.181	2.957
CH ₃ O-Br	1.983	2.135	NH ₂ -O	2.489	2.257
CH ₃ S-OCH ₃	2.741	2.893	CH ₃ CO-OCH ₃	4.408	4.163
B-C ₂ H ₅	3.671	3.823	SiH ₃ -NH ₂	4.474	4.723
SH-S	2.670	2.512	SiH ₃ -OCH ₃	4.804	5.065
S-C ₂ H ₅	3.114	2.951	SiH ₃ -C ₂ H ₅	3.661	3.93
Se-SCH ₃	2.527	2.358	CH ₃ O-O	1.866	1.589
HCC- <i>i</i> C ₃ H ₇	5.425	5.252	CH ₂ CH-O	4.454	4.162
HCC-C ₂ H ₅	5.448	5.270	C ₂ H ₅ -O	3.872	3.58
B-SCH ₃	3.821	3.633	B-NH ₂	4.938	4.642
CH ₃ CO-OH	4.740	4.547	B-OH	5.721	5.418
SiH ₃ -OH	5.287	5.481	HCC- <i>t</i> C ₄ H ₉	5.403	5.098
<i>t</i> C ₄ H ₉ -C ₂ H ₅	3.769	3.574	Si-SH	3.215	2.907
S-OCH ₃	2.897	2.700	HCC-S	4.564	4.249
HCC-SH	4.713	4.650	S-NH ₂	2.905	2.801
NH ₂ -OH	2.730	2.663	Se-CCH	4.157	4.047
P-OH	4.064	4.133	B-CH ₃	3.801	3.912
SiH ₃ -SH	3.753	3.823	CH ₂ CH-OH	4.734	4.619
S-CH ₃	3.085	3.012	CH ₂ CH-S	3.638	3.518
HS-F	3.548	3.622	HCC-CH ₃	5.471	5.350
P-CCH	4.473	4.549	HS-COCH ₃	3.214	3.336
<i>i</i> C ₃ H ₇ -C ₂ H ₅	3.808	3.722	CH ₂ CH- <i>t</i> C ₄ H ₉	4.299	4.177
SiH ₃ -CCH	5.540	5.628	SH-OCH ₃	2.662	2.785
CH ₃ O-F	1.992	1.900	CH ₃ -O	3.734	3.608
