Electronic Supplementary Information

Bond-Energy Decoupling: Principle and Application to Heterogeneous Catalysis

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Supplementary figures

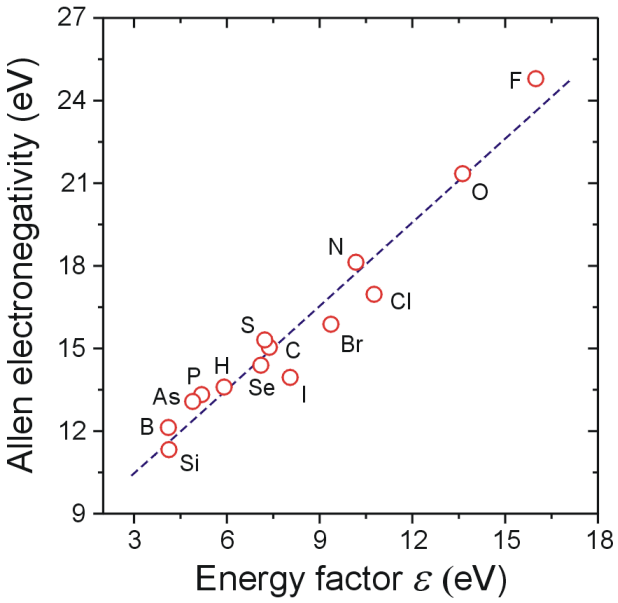

Figure S1 Correlation between the energy factor (ε) and the Allen electronegativity which represents the average energy of valence electrons.

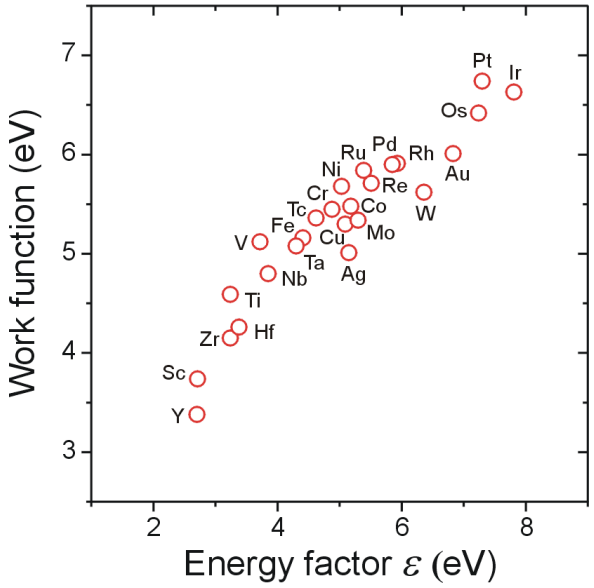

Figure S2 Correlation between the energy factor (ε) and the work function of 25 transition metal surfaces here studied (Table 1).

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	tC$_4$H$_9$-tC$_4$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
iC$_3$H$_7$-iC$_3$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-tC$_4$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$_3$-iC$_3$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-tC$_4$H$_9$	3.609
H-CCH	5.743	Br-P	2.798
F-tC$_4$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_6H_5	3.449	CH_3O-C_6H_5	4.303
Cl-SiH_3	4.709	HO-CH_3	3.952
C_6H_5-$CH_2C_6H_5$	3.939	Cl-C	3.366
CH_3CO-C_6H_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-$CH_2C_6H_5$	3.854	CH_3O-iC_3H_7	3.700
F-NH_2	2.932	Cl-$CH_2C_6H_5$	3.070
CH_3-tC_4H_9	3.730	H-NH_2	4.627
CH_3CO-tC_4H_9	3.375	HO-$CH_2C_6H_5$	3.425
CH_3O-tC_4H_9	3.622	CH_3-iC_3H_7	3.786
H-C_6F_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-iC_3H_7	4.217	Br-B	3.735
H-Se	3.319	Cl-O	2.065
tC_4H_9-SH	3.084	Cl-Br	2.235
Br-$CH_2C_6H_5$	2.442	CH_3-$CH_2C_6H_5$	3.331
H-C_2H_5	4.320	CH_3CO-C_2H_5	3.562
Cl-B	4.590	H-B	3.797
OH-C_6H_5	4.767	HO-iC_3H_7	4.086
Cl-C_6F_5	3.935	HO-tC_4H_9	4.090
H-I	3.053	F-CCH	5.365
NH_2-iC_3H_7	3.669	F-P	5.107
F-iC_3H_7	4.976	Cl-iC_3H_7	3.631
F-$C_6H_5CH_2$	4.240	Cl-CH_3	3.592
H-C_6H_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_3O-CH_3	3.609
F-SiH_3	6.574	H-SH	3.913
NH_2-CH_3	3.653	Br-iC_3H_7	3.063
CH_3-C_6F_5	4.515	Br-tC_4H_9	2.998
Cl-C_6H_5	4.104	I-SiH_3	3.061
Cl-C_2H_5	3.613	CH_3-C_6H_5	4.385
H-O	4.758	H-Br	3.757
NH_2-C_2H_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_2H_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_2H_5	3.800
HO-SCH_3	3.111	F-C_6H_5	5.408
F-C	4.533	H-SiH_3	3.939
Br-Si	2.959	Cl-P	3.392
NH_2-tC_4H_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	-tC_4H_9	6.363	0.369
-F	16.036	0.159	-C_6H_5	7.057	0.431
-Cl	10.768	0.242	-$CH_2C_6H_5$	7.169	0.317
-Br	9.373	0.231	-C_6F_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≡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_2H_5	7.211	0.368	-As	4.897	0.266
-iC_3H_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_2CH-iC_3H_7	4.342	4.341	Se-OH	3.000	2.973
CH_3S-$COCH_3$	3.280	3.276	S-$COCH_3$	2.924	2.892
CH_2CH-$COCH_3$	4.173	4.164	Se-NH_2	2.661	2.701
CH_2CH-CCH	6.006	6.019	CH_3S-tC_4H_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_3CO-O	4.182	4.167	iC_3H_7-OCH_3	3.830	3.775
CH_3S-O	2.851	2.833	CH_3O-Cl	2.146	2.201
SH-Br	2.419	2.441	B-$CHCH_2$	4.326	4.383
CH_3S-N	2.368	2.341	CH_2CH-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_3S-NH_2	2.864	3.067
CH_3S-OH	3.082	3.219	S-OH	3.227	3.016
SH-Cl	2.703	2.842	B-SH	3.944	3.732
CH_2CH-OCH_3	4.367	4.226	CH_3S-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_3O-Br	1.983	2.135	NH_2-O	2.489	2.257
CH_3S-OCH_3	2.741	2.893	CH_3CO-OCH_3	4.408	4.163
B-C_2H_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_2H_5	3.114	2.951	SiH_3-C_2H_5	3.661	3.93
Se-SCH_3	2.527	2.358	CH_3O-O	1.866	1.589
HCC-iC_3H_7	5.425	5.252	CH_2CH-O	4.454	4.162
HCC-C_2H_5	5.448	5.270	C_2H_5-O	3.872	3.58
B-SCH_3	3.821	3.633	B-NH_2	4.938	4.642
CH_3CO-OH	4.740	4.547	B-OH	5.721	5.418
SiH_3-OH	5.287	5.481	HCC-tC_4H_9	5.403	5.098
tC_4H_9-C_2H_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_2CH-OH	4.734	4.619
S-CH_3	3.085	3.012	CH_2CH-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
iC_3H_7-C_2H_5	3.808	3.722	CH_2CH-tC_4H_9	4.299	4.177
SiH_3-CCH	5.540	5.628	SH-OCH_3	2.662	2.785
CH_3O-F	1.992	1.900	CH_3-O	3.734	3.608