Supporting Information

Pattern Recognition Correlating Materials Properties of the Elements to Their Kinetics for the Hydrogen Evolution Reaction

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Experimental Procedure for Linear Sweep Voltammetry Experiments

Linear sweep voltammograms (LSV) were conducted to measure the exchange current density on $MoSi_2$. Commercial $MoSi_2$ powder (Stem Chemicals, Inc., Newburyport, MA) was used as the active material. The $MoSi_2$ powder was drop-cast onto a 3 mm diameter glassy carbon, GC, electrode (CH Instruments, Austin, TX) similar to a previously reported method.[1] Here, 5 mg of the $MoSi_2$ powder was mixed with 1 mg Vulcan Carbon (Cabot Corporation, Boston, MA), 20 µL of 5% Nafion solution (Sigma-Aldrich, St. Louis, MO), and 1 mL of ethanol. After sonicating the suspension for ~30 min, 20 µL of the suspension was drop-cast onto the GC electrode and was allowed to dry in a jar saturated with ethanol for at least 24 hr. The LSVs were performed using a CHI 630 potentiostat (CH Instruments, Austin, TX) in a custom-designed U-shaped three-compartment cell. The tests were conducted using 1 M $HClO_4$ and the electrolyte was deaerated with Ar for at least 15 min. The electrochemical cell was sealed with parafilm prior to running the experiment. The LSVs were conducted at 1 mV/s using a Ag/AgCl reference electrode and a W wire counter electrode to avoid any Pt contamination caused by the

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counter electrode. At least five forward and back cycles were performed to establish a constant current/potential curve for the $MoSi_2$ measurement, and shown is the last cycle for two separate experiments. Comparison LSVs on an uncoated GC disk electrode and a Pt disk electrode were also performed. To obtain the exchange current density, MathCAD was used to find best-fit values of j^0 and α when the experimental data is fit to the Tafel equation.

Supplemental Figures

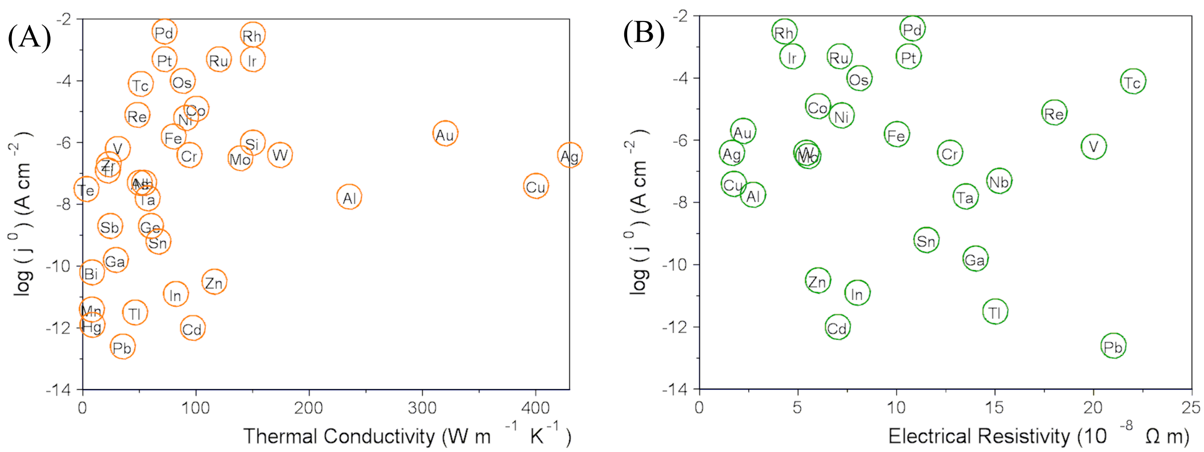

Figure S1. Log (j^0) for the hydrogen evolution reaction in acid vs. (A) thermal conductivity and (B) electrical resistivity for the elements. Thermal conductivity and electrical resistivity both resulted in low MIC values of 0.38 and 0.30 respectively, showing almost random correlations.

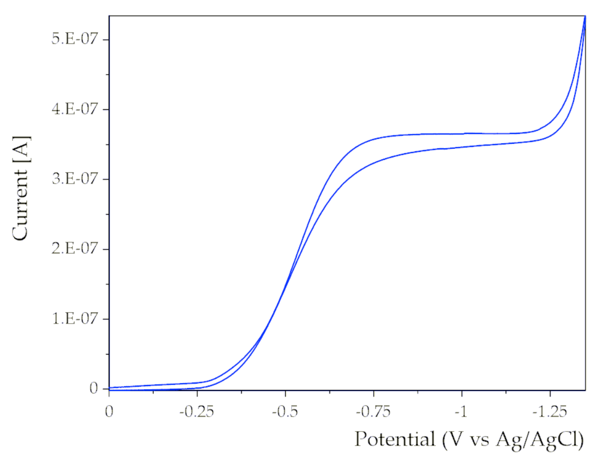

Figure S2. Cyclic voltammogram of a 25 μm Pt UME in a solution of 0.1 M NaCl + 0.01 M HCl at 50 mV/s. This demonstrates that hydrogen evolution can occur from both proton reduction (~-0.3 V vs. Ag/AgCl) and water reduction (~-1.25 V vs. Ag/AgCl).

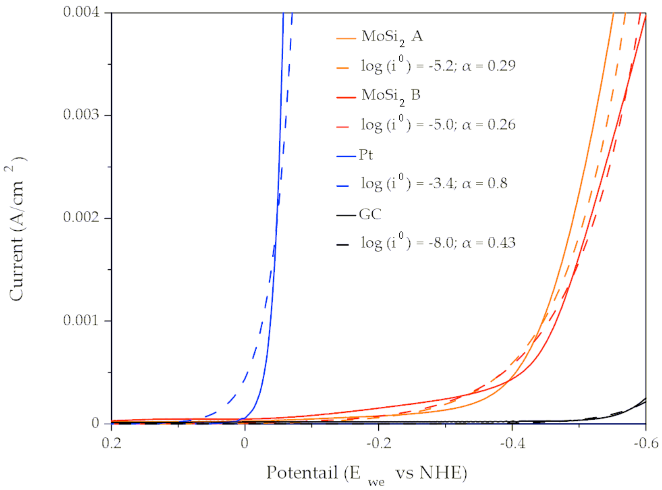

Figure S3. Linear sweep voltammograms of Pt disk electrode, a glassy carbon disk electrode, and two glassy carbon disk electrodes coated with $MoSi_2$ powder in a solution of 1 M $HClO_4$ at 1 mV/s. Also shown are best fit values for log (j^0) and α when the experimental data is fit to the Tafel equation.

Table S1: List of materials properties investigated in correlation studies with the exchange current density for hydrogen evolution in acid. Superscripts designate the source from which data was obtained.[2, 3, 4] Also shown is the MIC value designating the strength of the correlation using the original value for Mn.

Property	MIC	Property	MIC
Bulk Modulus/Gpa [2]	0.76161	Valence D-Orbital Radius (max)/pm [2]	0.43881
Melting Point/K [2]	0.70805	Number e- In Fifth Orbital [3]	0.42286
Enthalpy of Atomization/kJ mol^{-1} [2]	0.67805	Electronegativity [3]	0.41545
Valence P-Orbital Radius (max)/pm [2]	0.65485	Entropy/J deg^{-1} mol^{-1} [3]	0.41175
Boiling Point/K [2]	0.65357	Velocity of Sound/m s-^{1} [2]	0.40637
Boiling Point/C [3]	0.64859	Atom Radius/pm [3]	0.40253
Rigidity modulus/Gpa [2]	0.63552	Element Bond Length/pm [2]	0.39139
Enthalpy of Vaporization/kJ mol^{-1} [2]	0.62461	Thermal Conductivity/W m^{-1} K^{-1} [2]	0.38321
Valence F-Orbital Radius (max)/pm [2]	0.61751	Number e- In Last Orbital [3]	0.37644
Heat of Vaporization/kJ mol^{-1} [3]	0.60397	Poisson's Ratio [2]	0.36178
Radius-Metallic/pm [2]	0.57003	Electron Affinity/kJ mol^{-1} [2]	0.36126
Heat of Fusion/kJ mol^{-1} [3]	0.56485	Reflectivity/% [2]	0.35313
Linear Expansion Coefficient/10^6 K^{-1} [2]	0.55556	Hardness - Vickers/MN m^{-2} [2]	0.35277
Valence S-Orbital Radius (max)/pm [2]	0.55078	Superconductivity Temperature/K [2]	0.34243
Number e- In Sixth Orbital [3]	0.55034	Electronegativity/Pauling Scale [2]	0.34231
Young's Modulus/Gpa [2]	0.54625	Proton Transfer pK_1 [3]	0.31418
Hardness - Brinell/MN m^{-2} [2]	0.54356	Refractive Index [2]	0.31127
Enthalpy of Fusion/kJ mol^{-1} [2]	0.53653	Electrical resistivity/10^{-8} Ωm [2]	0.2993
Heat of Sublimation/kJ mol^{-1} [3]	0.52384	Ionic Radius (Pauling)/pm [2]	0.29354
Modulus of Elasticity/Gpa [4]	0.52277	Number e- In Fourth Orbital [3]	0.28584
Molar Volume/cm^3 [2]	0.50768	1st Ionization Energy/kJ mol^{-1} [3]	0.27404
Tensile Strength-Ultimate/MPa [4]	0.49343	Number e- In Third Orbital [3]	0.27394
Density/kg m^{-3} [2]	0.48479	Single Bond Radius/pm [3]	0.24884
Heat Capacity/J deg^{-1} mol^{-1} [3]	0.47706	Covalent Radius/pm [2]	0.23956
Mineralogical Hardness/Moh Scale [2]	0.47026	Van der Waals Radius/pm [2]	0.12369

Table S2: Ranking of the elements in order of highest to lowest exchange current densities for the hydrogen evolution reaction in acid. Also listed are the corresponding log (j^0), melting point (MP) and bulk modulus (BM). Highlighted elements fall within both optimum ranges (MP 1800 - 2750 K & MP >180 GPa).

Name	Rank	log (j^0)	MP (K)	BM (GPa)
Pd	1	-2.4	1828.05	180
Rh	2	-2.5	2237	380
Ir	3	-3.3	2739	320
Pt	4	-3.3	2041.4	230
Ru	5	-3.3	2607	220
Os	6	-4	3306	418
Tc	7	-4.1	2430	297
Mn	8	-4.5	1519	120
Co	9	-4.9	1768	180
Re	10	-5.1	3459	370
Ni	11	-5.2	1728	180
Au	12	-5.7	1337.33	220
Fe	13	-5.8	1811	170
Si	14	-6	1687	100
V	15	-6.2	2183	160
Ag	16	-6.4	1234.93	100
Cr	17	-6.4	2180	160
W	18	-6.4	3695	310
Mo	19	-6.5	2896	230
Zr	20	-6.7	2128	83.3
Ti	21	-6.9	1941	110
As	22	-7.3	1090	22
Nb	23	-7.3	2750	170
Cu	24	-7.4	1357.77	140
Te	25	-7.5	722.66	65
Al	26	-7.75	933.47	76
Ta	27	-7.8	3290	200
Ge	28	-8.7	1211.4	77.2
Sb	29	-8.7	903.78	42
Sn	30	-9.2	505.08	58
Ga	31	-9.8	302.91	56.9
Bi	32	-10.2	544.4	31
Zn	33	-10.5	692.68	70
In	34	-10.9	429.75	41.4
Tl	35	-11.5	577	43
Hg	36	-11.9	234.32	25
Cd	37	-12	594.22	42
Pb	38	-12.6	600.61	46

Supporting Information References

[1] Suntivich, J.; Gasteiger, H. A.; Yabuuchi, N.; Shao-Horn, Y., Electrocatalytic Measurement Methodology of Oxide Catalysts Using a Thin-Film Rotating Disk Electrode *J. Electrochm. Soc.* **2010**, *157*, B1263.

[2] Winter, M. WebElements: The Periodic Table on the Web. http://www.webelements.com (accessed Feb 8, 2012).

[3] *Lange's Handbook of Chemistry* 16th ed.; McGraw-Hill Professional Publishing: New York, NY, USA **2005**.

[4] Matweb Material Property Data. http://www.matweb.com (accessed Mar 8, 2012).