Supplementary Information

# Thermochemical Electronegativities of the Elements

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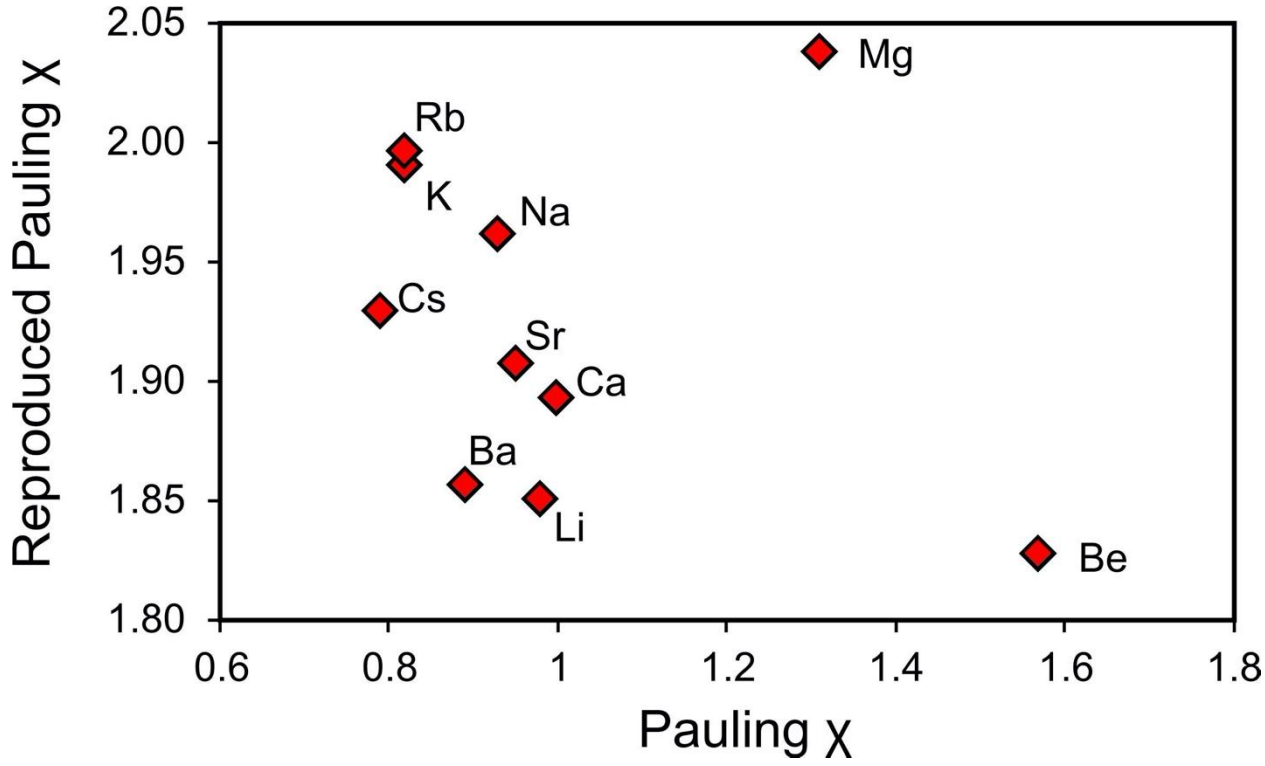
**Supplementary Figure 1.** Standard Pauling electronegativities (x-axis, in $eV^{-1/2}$) compared with Pauling electronegativities (y-axis, in $eV^{-1/2}$) calculated using experimental bond energies for alkali and alkali earth metals. One can see very large difference.



**Supplementary Table 2. Experimental bond dissociation energies used for calculating electronegativities.**

| Homonuclear bonds | Dissociation Enthalpy / (eV) | Heteronuclear bonds | Dissociation Enthalpy / (eV) |
|---|---|---|---|
| H2 | 4.517 | HF | 5.904 |
| Li2 | 1.116 | LiF | 6.001 |
| Be2 | 2.156 | BeF | 6.622 |
| B2 | 4.353 | F2B-F | 5.773 |
| C2H6 (C-C) | 3.911 | H3C-F | 4.770 |
| N2H4 (N-N) | 2.871 | H2N-H | 4.665 |
| H2O2 (O-O) | 2.183 | H-OH | 5.152 |
| F2 | 1.644 | | |
| Na2 | 0.796 | NaF | 5.379 |
| Mg2 | 1.337 | MgF | 5.343 |
| Al2 | 2.739 | AlF | 6.996 |
| H3Si-SiH3 (Si-Si) | 3.327 | SiF | 5.974 |
| H2P-PH2 (P-P) | 2.654 | H2P-H | 3.638 |
| FS-SF (S-S) | 3.755 | SF | 3.560 |
| Cl2 | 2.514 | HCl | 4.471 |
| K2 | 0.528 | KF | 5.127 |
| Ca2 | 1.088 | CaF | 5.807 |
| Sc2 | 1.689 | ScF | 6.209 |
| Ti2 | 1.219 | TiF | 5.897 |
| V2 | 0.961 | VF | 6.115 |
| Cr2 | 0.742 | CrF | 5.421 |
| Mn2 | 0.532 | MnF | 4.614 |
| Fe2 | 0.778 | FeF | 4.633 |
| Co2 | 0.740 | CoF | 4.467 |

| | | | |
|---|---|---|---|
| Ni2 | 0.741 | NiF | 4.557 |
| Cu2 | 2.083 | CuF | 4.291 |
| Zn2 | 0.230 | ZnF | 3.773 |
| Ga2 | 1.197 | GaF | 4.941 |
| Ge2 | 2.740 | GeF | 5.421 |
| As2 | 3.999 | AsF | 4.249 |
| Se2 | 1.769 | SeF | 3.513 |
| Br2 | 2.056 | FBr | 2.637 |
| Rb2 | 0.503 | RbF | 5.091 |
| Sr2 | 0.871 | SrF | 5.638 |
| Y2 | 2.798 | YF | 7.103 |
| Zr2 | 1.052 | ZrF | 6.500 |
| Nb2 | 1.349 | NbF | 4.480 |
| Mo2 | 1.227 | MoF | 4.809 |
| Tc2 | 0.050 | TcF | 2.020 |
| Ru2 | 1.125 | RuF | 3.781 |
| Rh2 | 0.963 | RhF | 3.686 |
| Pd2 | 0.644 | PdF | 3.088 |
| Ag2 | 1.631 | AgF | 3.699 |
| Cd2 | 0.076 | CdF | 3.161 |
| In2 | 1.036 | InF | 5.244 |
| Sn2 | 1.939 | SnF | 4.933 |
| Sb2 | 3.127 | SbF | 4.550 |
| Te2 | 2.860 | | |
| I2 | 1.681 | FI | 2.730 |
| Cs2 | 0.433 | CsF | 5.327 |
| Ba2 | 0.698 | BaF | 5.767 |

| | | | |
|---|---|---|---|
| Hf2 | 1.070 | HfF | 6.737 |
| Ta2 | 1.469 | TaF | 5.939 |
| W2 | 1.594 | WF | 5.638 |
| Re2 | 1.340 | ReF | 4.458 |
| Os2 | 1.364 | OsF | 3.955 |
| Ir2 | 1.149 | IrF | 3.430 |
| Pt2 | 0.980 | PtF | 2.684 |
| Au2 | 2.294 | AuCl | 3.555 |
| Hg2 | 0.084 | HgF | 1.866 |
| Tl2 | 0.616 | TlF | 4.550 |
| Pb2 | 0.898 | PbF | 3.679 |
| Fr2 | 0.430 | FrF | 5.160 |
| La2 | 2.520 | LaF | 6.830 |
| Ce2 | 2.470 | CeF | 6.032 |
| Pr2 | 1.310 | PrF | 6.032 |
| Nd2 | 0.830 | NdF | 5.651 |
| Sm2 | 0.520 | SmF | 5.856 |
| Eu2 | 0.300 | EuF | 5.638 |
| Gd2 | 1.780 | GdF | 6.115 |
| Tb2 | 1.320 | TbF | 5.814 |
| Dy2 | 0.690 | DyF | 5.503 |
| Ho2 | 0.820 | HoF | 5.597 |
| Er2 | 0.740 | ErF | 5.856 |
| Tm2 | 0.520 | TmF | 5.286 |
| Yb2 | 0.170 | YbF | 5.365 |
| Lu2 | 1.430 | LuF | 4.198 |
| Th2 | 2.995 | ThF | 6.758 |

| | | | |
|---|---|---|---|
| U2 | 2.301 | UF | 6.716 |
| - | - | LiCl | 4.710 |
| - | - | NaCl | 4.384 |
| - | - | KCl | 4.405 |
| - | - | RbCl | 4.474 |
| - | - | CsCl | 4.619 |
| - | - | LiBr | 4.195 |
| - | - | NaBr | 3.900 |
| - | - | KBr | 3.929 |
| - | - | RbBr | 3.946 |
| - | - | CsBr | 4.033 |
| - | - | LiI | 3.534 |
| - | - | NaI | 3.196 |
| - | - | KI | 3.343 |
| - | - | RbI | 3.304 |
| - | - | CsI | 3.508 |

**Supplementary Table 3**. Electronegativities of the elements from different scales. For Martinov-Batsanov scale there are different electronegativity values for the different oxidation states (reported in brackets) of each element.

| Element | Pauling / $(eV^{-1/2})$ | Mulliken / $(eV)$ | Allen / $(eV)$ | Martynov & Batsanov / $(eV^{-1/2})$ | Our scale |
|---|---|---|---|---|---|
| H | 2.20 | 7.18 | 2.3 | - | 3.04 |
| Li | 0.98 | 3.00 | 0.912 | 0.95 | 2.17 |
| Na | 0.93 | 2.84 | 0.869 | 0.9 | 2.15 |
| K | 0.82 | 2.42 | 0.734 | 0.8 | 2.07 |
| Rb | 0.82 | 2.33 | 0.706 | 0.8 | 2.07 |
| Cs | 0.79 | 2.18 | 0.659 | 0.75 | 1.97 |
| Fr | 0.70 | 2.21 | 0.67 | 0.7 | 2.01 |
| Be | 1.57 | 4.41 | 1.576 | 1.5 | 2.42 |
| Mg | 1.31 | 3.62 | 1.293 | 1.2 | 2.39 |
| Ca | 1.00 | 3.07 | 1.034 | 1 | 2.20 |
| Sr | 0.95 | 2.87 | 0.963 | 1 | 2.13 |
| Ba | 0.89 | 2.68 | 0.881 | 0.9 | 2.02 |
| Ra | 0.90 | 2.69 | 0.89 | 0.9 | - |
| Sc | 1.36 | 3.37 | 1.19 | 1.3 | 2.35 |
| Ti | 1.54 | 3.45 | 1.38 | 1.6 | 2.23 |
| V | 1.63 | 3.64 | 1.53 | (II) 1.5 (III) 1.7 (V) 2.00 | 2.08 |
| Cr | 1.66 | 3.72 | 1.65 | (II) 1.6 (III) 1.8 (V) 2.2 | 2.12 |
| Mn | 1.55 | 3.46 | 1.75 | (II) 1.5 (III) 1.8 (IV) 2.0 (VII) 2.3 | 2.20 |
| Fe | 1.83 | 4.03 | 1.8 | (II) 1.8 (III) 1.9 | 2.32 |
| Co | 1.88 | 4.27 | 1.84 | (II) 1.8 (III) 2.0 (IV) 3.1 | 2.34 |
| Ni | 1.91 | 4.40 | 1.88 | (II) 1.9 (III) 2.0 (IV) 3.4 | 2.32 |
| Cu | 1.90 | 4.48 | 1.85 | (I) 1.8) (II) 2.1 | 2.86 |
| Zn | 1.65 | 4.40 | 1.59 | 1.6 | 2.26 |
| Y | 1.22 | 3.26 | 1.12 | 1.25 | 2.52 |
| Zr | 1.33 | 3.53 | 1.32 | 1.5 | 2.05 |
| Nb | 1.60 | 3.84 | 1.41 | (III) 1.6 (V) 1.9 | 2.59 |
| Mo | 2.16 | 3.92 | 1.47 | (IV) 1.8 (VI) 2.2 | 2.47 |
| Tc | 1.90 | 3.91 | 1.51 | (IV) 1.9 | 2.82 |

| | | | | | |
|---|---|---|---|---|---|
| Ru | 2.20 | 4.20 | 1.54 | (II) 2.0 (III) 2.0 (IV) 2.1 | 2.68 |
| Rh | 2.28 | 4.30 | 1.56 | (II) 2.1 (III) 2.1 | 2.65 |
| Pd | 2.20 | 4.45 | 1.58 | (II) 2.2 (III) 2.2 (IV) 2.3 | 2.70 |
| Ag | 1.93 | 4.44 | 1.87 | 1.9 | 2.88 |
| Cd | 1.69 | 4.14 | 1.52 | 1.7 | 2.36 |
| Hf | 1.30 | 3.50 | 1.16 | 1.4 | 2.01 |
| Ta | 1.50 | 4.10 | 1.34 | (III) 1.5 (V) 1.8 | 2.32 |
| W | 2.36 | 4.40 | 1.47 | (IV) 1.8 (V) 2.1 | 2.42 |
| Re | 1.90 | 3.97 | 1.6 | (IV) 1.9 | 2.59 |
| Os | 2.20 | 4.89 | 1.65 | (II) 2.0 (III) 2.1 (IV) 2.2 | 2.72 |
| Ir | 2.20 | 5.34 | 1.68 | (II) 2.1 (III) 2.2 | 2.79 |
| Pt | 2.28 | 5.57 | 1.72 | (II) 2.3 (III) 2.3 (IV) 2.4 | 2.98 |
| Au | 2.54 | 5.77 | 1.92 | (I) 2.0 (III) 2.4 | 2.81 |
| Hg | 2.00 | 4.97 | 1.76 | 1.8 | 2.92 |
| B | 2.04 | 4.29 | 2.05 | 1.9 | 3.04 |
| Al | 1.61 | 3.21 | 1.613 | 1.5 | 2.52 |
| Ga | 1.81 | 3.21 | 1.756 | 1.7 | 2.43 |
| In | 1.78 | 3.09 | 1.656 | 1.8 | 2.29 |
| Tl | 1.62 | 3.24 | 1.789 | (I) 1.4 (III) 1.9 | 2.26 |
| C | 2.55 | 6.26 | 2.544 | 2.5 | 3.15 |
| Si | 1.90 | 4.77 | 1.916 | 1.9 | 2.82 |
| Ge | 2.01 | 4.57 | 1.994 | 2.0 | 2.79 |
| Sn | 1.96 | 4.23 | 1.824 | (II) 1.8 (IV) 2.0 | 2.68 |
| Pb | 2.33 | 3.89 | 1.854 | (II) 1.9 (IV) 2.1 | 2.62 |
| N | 3.04 | 7.23 | 3.066 | 3.0 | 3.56 |
| P | 2.19 | 5.62 | 2.253 | 2.1 | 3.16 |
| As | 2.18 | 5.31 | 2.211 | 2.0 | 3.15 |
| Sb | 2.05 | 4.85 | 1.984 | (III) 1.9 (V) 2.2 | 3.05 |
| Bi | 2.02 | 4.11 | 2.01 | (III) 1.9 (V) 2.2 | - |
| O | 3.44 | 7.54 | 3.61 | 3.55 | 3.78 |
| S | 2.58 | 6.22 | 2.589 | 2.5 | 3.44 |
| Se | 2.55 | 5.89 | 2.424 | 2.4 | 3.37 |

| | | | | | |
|---|---|---|---|---|---|
| Te | 2.10 | 5.49 | 2.158 | 2.1 | 3.14 |
| Po | 2.00 | 4.91 | 2.19 | 2.0 | - |
| F | 3.98 | 10.41 | 4.193 | 4.0 | 4.00 |
| Cl | 3.16 | 8.29 | 2.869 | 3.0 | 3.56 |
| Br | 2.96 | 7.59 | 2.685 | 2.8 | 3.45 |
| I | 2.66 | 6.76 | 2.359 | 2.5 | 3.20 |
| At | 2.20 | 5.87 | 2.39 | 2.2 | - |
| La | 1.10 | 3.06 | - | 1.2 | 2.49 |
| Ce | 1.12 | 3.05 | - | - | 2.61 |
| Pr | 1.13 | 3.21 | - | - | 2.24 |
| Nd | 1.14 | 3.72 | - | - | 2.11 |
| Pm | 1.13 | 2.86 | - | - | - |
| Sm | 1.17 | 2.90 | - | - | 1.90 |
| Eu | 1.20 | 2.89 | - | - | 1.81 |
| Gd | 1.20 | 3.14 | - | - | 2.40 |
| Tb | 1.10 | 3.51 | - | - | 2.29 |
| Dy | 1.22 | 3.15 | - | - | 2.07 |
| Ho | 1.23 | 3.18 | - | - | 2.12 |
| Er | 1.24 | 3.21 | - | - | 2.02 |
| Tm | 1.25 | 3.61 | - | - | 2.03 |
| Yb | 1.10 | 3.12 | - | - | 1.78 |
| Lu | 1.27 | 2.89 | 1.09 | - | 2.68 |
| Th | 1.30 | 3.63 | - | (IV) 1.3 | 2.62 |
| U | 1.38 | 3.36 | - | (IV) 1.4 (V) 1.6 (VI) 1.8 | 2.45 |
| He | - | 12.29 | 4.16 | - | - |
| Ne | - | 10.78 | 4.787 | - | - |
| Ar | - | 7.88 | 3.242 | - | - |
| Kr | 3.23 | 7.00 | 2.966 | - | - |
| Xe | 3.02 | 6.07 | 2.582 | - | - |
| Rn | 2.81 | 5.37 | 2.6 | - | - |

**Supplementary Table 4. Lattice parameters of the crystal structures used for Bader charge calculations.**

| System | Space Group | $a$ / (Å) | $b$ / (Å) | $c$ / (Å) | $\alpha$ | $\beta$ | $\gamma$ |
|---|---|---|---|---|---|---|---|
| $Al_2O_3$ | $R\bar{3}c$ | 4.803 | 4.803 | 13.110 | 90.00 | 90.00 | 120.00 |
| AlN | $P6_3mc$ | 3.127 | 3.127 | 5.013 | 90.00 | 90.00 | 120.00 |
| $AuB_2$ | $P6/mmm$ | 3.005 | 3.005 | 4.281 | 90.00 | 90.00 | 120.00 |
| MoB | $I4_1/amd$ | 3.127 | 3.127 | 17.007 | 90.00 | 90.00 | 90.00 |
| WB | $I4_1/amd$ | 3.139 | 3.139 | 16.947 | 90.00 | 90.00 | 90.00 |
| $Bi_2Te_3$ | $R\bar{3}m$ | 4.444 | 4.444 | 31.484 | 90.00 | 90.00 | 120.00 |
| LiH | $Fm\bar{3}m$ | 2.841 | 2.841 | 2.841 | 60.00 | 60.00 | 60.00 |
| $PtH_4$ | $Im\bar{3}m$ | 6.711 | 6.711 | 6.711 | 90.00 | 90.00 | 90.00 |
| PbH | $P6_3mc$ | 3.514 | 3.514 | 7.369 | 90.00 | 90.00 | 120.00 |
| RhH | $Fm\bar{3}m$ | 4.043 | 4.043 | 4.043 | 90.00 | 90.00 | 90.00 |
| BaO | $Fm\bar{3}m$ | 5.601 | 5.601 | 5.601 | 90.00 | 90.00 | 90.00 |
| BeO | $P6_3mc$ | 2.702 | 2.702 | 4.389 | 90.00 | 90.00 | 120.00 |
| MgO | $Fm\bar{3}m$ | 4.248 | 4.248 | 4.248 | 90.00 | 90.00 | 90.00 |
| LiF | $Fm\bar{3}m$ | 4.072 | 4.072 | 4.072 | 90.00 | 90.00 | 90.00 |
| LiCl | $Fm\bar{3}m$ | 3.643 | 3.643 | 3.643 | 60.00 | 60.00 | 60.00 |
| LiI | $P6_3mc$ | 4.261 | 4.261 | 4.261 | 60.00 | 60.00 | 60.00 |
| NaF | $Fm\bar{3}m$ | 3.321 | 3.321 | 3.321 | 90.00 | 90.00 | 90.00 |
| NaCl | $Fm\bar{3}m$ | 5.696 | 5.696 | 5.696 | 90.00 | 90.00 | 90.00 |
| NaI | $Fm\bar{3}m$ | 6.532 | 6.532 | 6.532 | 90.00 | 90.00 | 90.00 |
| CsF | $Fm\bar{3}m$ | 4.326 | 4.326 | 4.326 | 60.00 | 60.00 | 60.00 |
| CsCl | $Fm\bar{3}m$ | 7.087 | 7.087 | 7.087 | 90.00 | 90.00 | 90.00 |
| CsI | $Fm\bar{3}m$ | 5.557 | 5.557 | 5.557 | 60.00 | 60.00 | 60.00 |
| $BeF_2$ | $I\bar{4}3m$ | 8.561 | 8.561 | 8.561 | 90.00 | 90.00 | 90.00 |
| $BeCl_2$ | $Ibam$ | 5.247 | 5.738 | 6.586 | 115.82 | 113.47 | 90.00 |
| $BeI_2$ | $Ibam$ | 6.505 | 6.143 | 7.554 | 113.99 | 115.50 | 90.00 |
| $MgF_2$ | $Ibam$ | 3.094 | 4.686 | 4.703 | 90.00 | 90.00 | 90.00 |
| $MgCl_2$ | $R\bar{3}m$ | 6.908 | 6.908 | 6.908 | 30.86 | 30.86 | 30.86 |
| MgI2 | $P\bar{3}m1$ | 4.210 | 4.210 | 7.731 | 90.00 | 90.00 | 120.00 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| $BaF_2$ | $Fm\underline{3}m$ | 4.442 | 4.442 | 4.442 | 60.00 | 60.00 | 60.00 |
| $BaCl_2$ | $Fm\underline{3}m$ | 5.242 | 5.242 | 5.242 | 60.00 | 60.00 | 60.00 |
| $BaI_2$ | $Pnma$ | 5.418 | 10.848 | 18.051 | 90.16 | 90.00 | 90.00 |
| KBr | $Fm\underline{3}m$ | 4.749 | 4.749 | 4.749 | 60.00 | 60.00 | 60.00 |
| SiC | $P6_3mc$ | 3.093 | 3.093 | 15.178 | 90.00 | 90.00 | 120.00 |
| $SiO_2$ (quartz) | $I\underline{4}2d$ | 5.036 | 5.036 | 7.371 | 90.00 | 90.00 | 90.00 |
| $TiO_2$ | $\frac{C2}{c}$ | 3.803 | 3.803 | 9.734 | 90.00 | 90.00 | 90.00 |
| ZnS (sphalerite) | $F\underline{4}3m$ | 5.431 | 5.431 | 5.431 | 90.00 | 90.00 | 90.00 |

**Supplementary Table 5.** Bader charges and degrees of ionicity in some molecules determined from experimental dipole moments, from Bader analysis, and calculated using Pauling's and our formulae.

| | Bader Charges | | Ionic Character / % | | | |
|---|---|---|---|---|---|---|
| System | Cation | Anion | From dipole moment | From Bader analysis | From Pauling's formula | From our formula |
| HF | 0.72 | -0.72 | 41.33 | 71.62 | 54.71 | 45.90 |
| HCl | 0.38 | -0.38 | 17.64 | 37.67 | 20.58 | 13.16 |
| HBr | 0.42 | -0.42 | 12.18 | 42.06 | 13.45 | 10.60 |
| HI | 0.44 | -0.44 | 5.80 | 43.56 | 5.15 | 1.69 |
| LiF | 0.70 | -0.70 | 83.66 | 69.82 | 89.46 | 89.28 |
| LiCl | 0.71 | -0.71 | 72.99 | 71.19 | 69.52 | 69.25 |
| LiBr | 0.79 | -0.79 | 69.34 | 79.28 | 62.47 | 66.45 |
| LiI | 0.84 | -0.84 | 54.68 | 84.14 | 50.62 | 50.70 |
| NaF | 0.63 | -0.63 | 87.82 | 62.87 | 90.23 | 89.79 |
| KCl | 0.88 | -0.88 | 79.94 | 88.25 | 74.56 | 74.42 |
| KBr | 0.90 | -0.90 | 78.26 | 89.98 | 68.17 | 71.91 |
| KI | 0.90 | -0.90 | 75.49 | 90.14 | 57.10 | 57.31 |
| CsF | 0.73 | -0.73 | 69.87 | 72.82 | 92.15 | 93.59 |

| | | | | | | |
|---|---|---|---|---|---|---|
| CsCl | 0.80 | -0.80 | 74.51 | 80.23 | 75.44 | 79.00 |
| CsI | 0.85 | -0.85 | 76.00 | 85.04 | 58.28 | 63.53 |
| ICl | 0.03 | -0.03 | 11.12 | 3.16 | 6.06 | 5.82 |
| IBr | 0.10 | -0.10 | 6.22 | 9.82 | 2.22 | 4.08 |

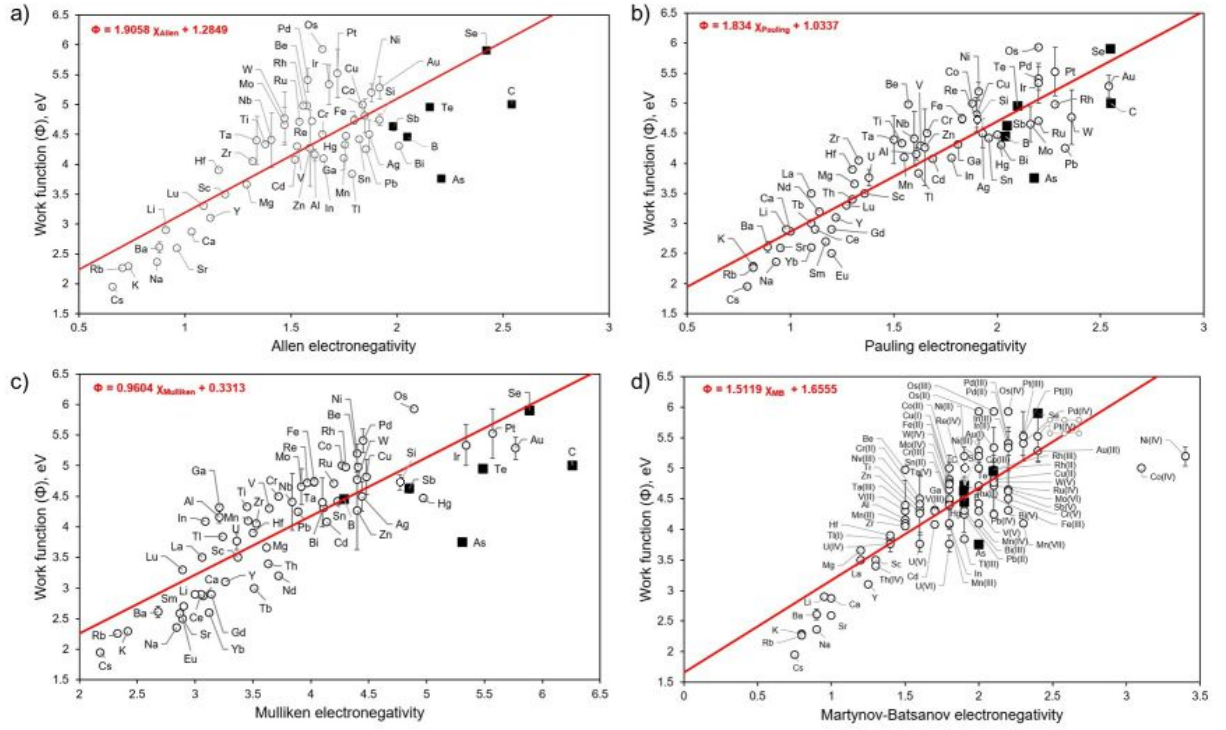
**Supplementary Table 6.** Bader charges and degrees of ionicity of some crystals determined using Bader analysis and calculated using Pauling's and our formulae.

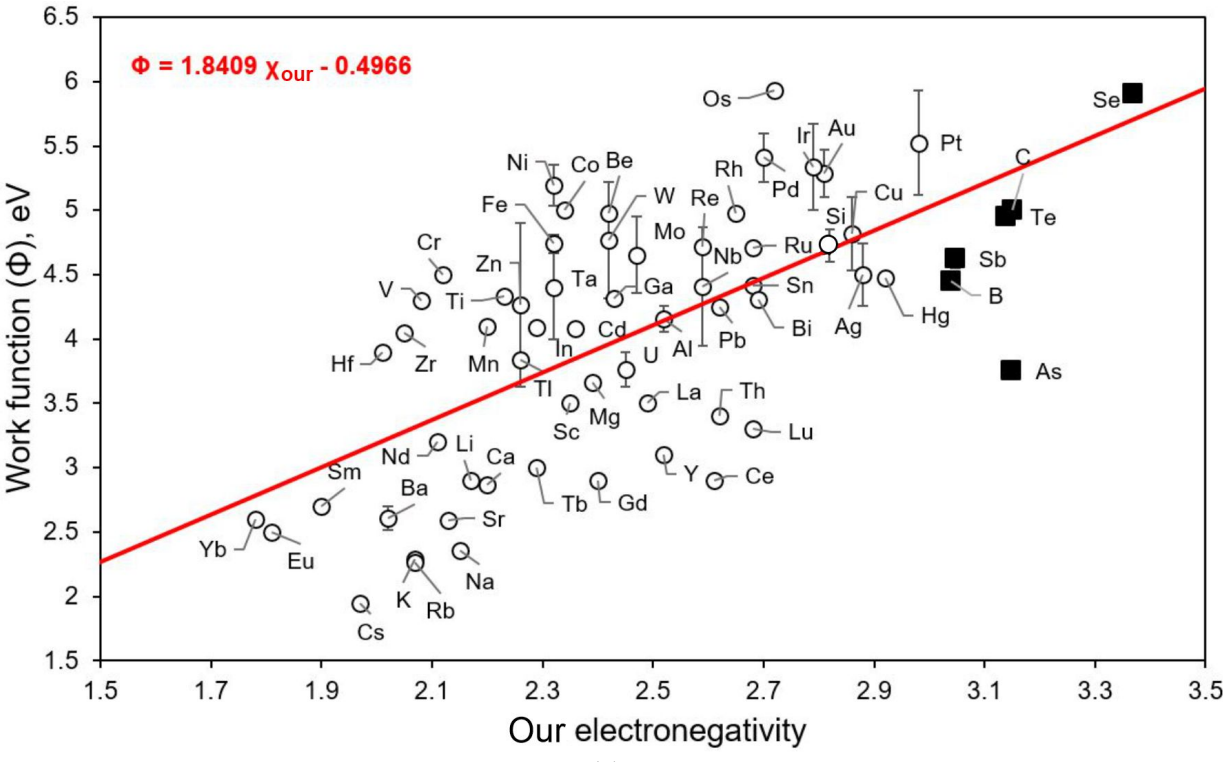
| | Bader Charges | | Ionic Character / % | | |
|---|---|---|---|---|---|
| System | Cation | Anion | From Bader analysis | From Pauling's formula | From our formula |
| AlN | 2.37 | -2.37 | 78.93 | 40.02 | 51.38 |
| $Al_2O_3$ | 2.48 | -1.65 | 82.62 | 56.71 | 65.30 |
| $BaF_2$ | 1.72 | -0.86 | 86.07 | 90.81 | 92.67 |
| $BaCl_2$ | 1.62 | -0.81 | 80.38 | 72.42 | 76.78 |
| $BaI_2$ | 1.55 | -0.78 | 77.71 | 54.31 | 60.48 |
| BaO | 1.56 | -1.56 | 78.18 | 80.32 | 87.32 |
| $BeF_2$ | 1.76 | -0.88 | 87.89 | 76.59 | 81.07 |
| $BeCl_2$ | 1.67 | -0.83 | 83.29 | 46.85 | 54.05 |
| $BeI_2$ | 1.54 | -0.77 | 76.79 | 25.70 | 33.34 |
| BeO | 1.69 | -1.69 | 84.45 | 58.28 | 70.86 |
| $Bi_2Te_3$ | 0.70 | -0.47 | 23.49 | 0.16 | 12.63 |
| CsF | 0.88 | -0.88 | 88.13 | 92.15 | 93.59 |
| CsCl | 0.84 | -0.84 | 84.29 | 75.44 | 79.00 |

| | | | | | |
|---|---|---|---|---|---|
| CsI | 0.81 | -0.81 | 80.69 | 58.28 | 63.53 |
| KBr | 0.83 | -0.83 | 82.90 | 68.17 | 71.91 |
| LiH | 0.83 | -0.83 | 83.23 | 31.07 | 39.63 |
| LiF | 0.87 | -0.87 | 86.82 | 89.46 | 89.28 |
| LiCl | 0.89 | -0.89 | 88.51 | 69.52 | 69.25 |
| LiI | 0.88 | -0.88 | 88.28 | 50.62 | 50.70 |
| $MgF_2$ | 1.67 | -0.84 | 83.53 | 83.17 | 82.24 |
| $MgCl_2$ | 1.66 | -0.83 | 82.84 | 57.50 | 56.02 |
| $MgI_2$ | 1.58 | -0.79 | 79.19 | 36.59 | 35.43 |
| MgO | 1.64 | -1.64 | 82.19 | 67.83 | 72.42 |
| NaF | 0.82 | -0.82 | 82.43 | 90.23 | 89.79 |
| NaCl | 0.83 | -0.83 | 82.91 | 71.15 | 70.33 |
| NaI | 0.82 | -0.82 | 82.40 | 52.68 | 52.05 |
| PbH | 0.37 | -0.37 | 37.40 | 2.69 | 11.09 |
| RhH | 0.10 | -0.10 | 9.61 | 0.16 | 9.64 |
| SiC | 2.64 | -2.64 | 66.10 | 10.02 | 7.00 |
| $SiO_2$ (quartz) | 3.22 | -1.61 | 80.45 | 44.73 | 45.90 |

| | | | | | |
|---|---|---|---|---|---|
| $TiO_2$ | 1.98 | -0.99 | 49.54 | 59.44 | 79.84 |
| ZnS (sphalerite) | 0.88 | -0.88 | 43.97 | 19.44 | 60.48 |

**Supplementary Figure 7** Correlation between different electronegativities with work function[7] of pure elements. *Legend*: metals, empty circles; non-metals, full squares.




(e)