Supporting Materials

# Extension of the Polarizable Charge Equilibration Model to Higher Oxidation States with Applications to Ge, As, Se, Br, Sn, Sb, Te, I, Pb, Bi, Po, and At Elements

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## 1. Parameter Set for PQEq2

Table S1: The electronegativity $\chi$, idempotential $J$, shell charge $Q_c$, atomic covalent radius $R_c=R_s$, and spring force constant $K_s$ for PQEq2.

| Atom | $\chi$ (eV) | J (eV) | $Q_c$ | $R_c=R_s$ (Å) | $K_s$ (kcal/mol/Å$^2$) |
|---|---|---|---|---|---|
| H | 4.52719 | 15.17433 | 1 | 0.371 | 2037.201 |
| He | 9.66 | 29.84 | 1 | 1.3 | 1619.411 |
| Li | 3.006 | 4.772 | 1 | 1.557 | 13.64832 |
| Be | 4.877 | 8.886 | 1 | 1.24 | 59.29709 |
| B | 5.11 | 9.5 | 1 | 0.822 | 109.592 |
| C | 5.41477 | 10.25602 | 1 | 0.759 | 198.8405 |
| N | 6.87577 | 10.26467 | 1 | 0.715 | 301.8761 |
| O | 9.7139 | 14.66128 | 1 | 0.669 | 414.0445 |
| F | 9.71494 | 17.7886 | 1 | 0.706 | 596.1646 |
| Ne | 11.04 | 21.1 | 1 | 1.768 | 842.1173 |
| Na | 2.843 | 4.592 | 1 | 2.085 | 13.77286 |
| Mg | 3.951 | 7.386 | 1 | 1.5 | 31.32676 |
| Al | 4.06 | 7.18 | 1 | 1.201 | 48.8329 |

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|---|---|---|---|---|---|
| Si | 4.80466 | 6.71377 | 1 | 1.176 | 60.04769 |
| P | 6.02536 | 7.86352 | 1 | 1.102 | 91.4776 |
| S | 7.01035 | 8.95326 | 1 | 1.047 | 114.5047 |
| Cl | 7.81003 | 10.23353 | 1 | 0.994 | 152.3228 |
| Ar | 9.465 | 12.71 | 1 | 2.108 | 202.3422 |
| K | 2.421 | 3.84 | 1 | 2.586 | 7.71165 |
| Ca | 3.231 | 5.76 | 1 | 2 | 14.5642 |
| Sc | 3.395 | 6.16 | 1 | 1.75 | 18.65526 |
| Ti | 3.47 | 6.76 | 1 | 1.607 | 22.74409 |
| V | 3.65 | 6.82 | 1 | 1.47 | 26.77933 |
| Cr | 3.415 | 7.73 | 1 | 1.402 | 28.62618 |
| Mn | 3.325 | 8.21 | 1 | 1.533 | 35.32593 |
| Fe | 3.76 | 8.28 | 1 | 1.393 | 39.53139 |
| Co | 4.105 | 8.35 | 1 | 1.406 | 44.27516 |
| Ni | 4.465 | 8.41 | 1 | 1.398 | 48.8329 |
| Cu | 3.729 | 5.002 | 1 | 1.434 | 53.55866 |

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|---|---|---|---|---|---|
| Zn | 5.106 | 8.57 | 1 | 1.4 | 57.75021 |
| Ga | 3.641 | 6.32 | 1 | 1.211 | 40.89454 |
| Ge | 4.80386 | 6.71243 | 1 | 1.189 | 56.86022 |
| As | 5.41473 | 7.5831 | 1 | 1.204 | 77.04494 |
| Se | 6.05692 | 8.40969 | 1 | 1.224 | 88.08056 |
| Br | 7.79 | 8.79002 | 1 | 1.141 | 108.8733 |
| Kr | 8.505 | 11.43 | 1 | 2.27 | 133.6595 |
| Rb | 2.331 | 3.692 | 1 | 2.77 | 7.02929 |
| Sr | 3.024 | 4.88 | 1 | 2.415 | 12.03129 |
| Y | 3.83 | 5.62 | 1 | 1.998 | 14.62836 |
| Zr | 3.4 | 7.1 | 1 | 1.758 | 18.55104 |
| Nb | 3.55 | 6.76 | 1 | 1.603 | 21.15055 |
| Mo | 3.465 | 7.51 | 1 | 1.53 | 25.94248 |
| Tc | 3.29 | 7.98 | 1 | 1.5 | 29.12839 |
| Ru | 3.575 | 8.03 | 1 | 1.5 | 34.58997 |
| Rh | 3.975 | 8.01 | 1 | 1.509 | 38.61206 |

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|---|---|---|---|---|---|
| Pd | 4.32 | 8 | 1 | 1.544 | 69.17994 |
| Ag | 4.436 | 6.268 | 1 | 1.622 | 48.97695 |
| Cd | 5.034 | 7.914 | 1 | 1.6 | 45.11735 |
| In | 3.506 | 5.792 | 1 | 1.404 | 32.55526 |
| Sn | 4.62392 | 6.45025 | 1 | 1.354 | 52.87639 |
| Sb | 4.56949 | 6.45124 | 1 | 1.404 | 50.31268 |
| Te | 6.02877 | 6.80311 | 1 | 1.38 | 60.37522 |
| I | 6.1548 | 7.50909 | 1 | 1.333 | 62.06798 |
| Xe | 7.595 | 9.95 | 1 | 2.459 | 82.11269 |
| Cs | 2.183 | 3.422 | 1 | 2.984 | 5.58842 |
| Ba | 2.814 | 4.792 | 1 | 2.442 | 8.36432 |
| La | 2.8355 | 5.483 | 1 | 2.071 | 10.67729 |
| Ce | 2.774 | 5.384 | 1 | 1.925 | 11.21837 |
| Pr | 2.858 | 5.128 | 1 | 2.007 | 11.77531 |
| Nd | 2.8685 | 5.241 | 1 | 2.007 | 10.57528 |
| Pm | 2.881 | 5.346 | 1 | 2 | 11.03202 |

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|---|---|---|---|---|---|
| Sm | 2.9115 | 5.439 | 1 | 1.978 | 11.52999 |
| Eu | 2.8785 | 5.575 | 1 | 2.227 | 11.98786 |
| Gd | 3.1665 | 5.949 | 1 | 1.968 | 14.13037 |
| Tb | 3.018 | 5.668 | 1 | 1.954 | 13.02211 |
| Dy | 3.0555 | 5.743 | 1 | 1.934 | 13.55362 |
| Ho | 3.127 | 5.782 | 1 | 1.925 | 14.0705 |
| Er | 3.1865 | 5.829 | 1 | 1.915 | 14.62836 |
| Tm | 3.2514 | 5.8658 | 1 | 2 | 15.23228 |
| Yb | 3.2889 | 5.93 | 1 | 2.158 | 15.88822 |
| Lu | 2.9629 | 4.9258 | 1 | 1.896 | 15.16273 |
| Hf | 3.7 | 6.8 | 1 | 1.759 | 20.49776 |
| Ta | 5.1 | 5.7 | 1 | 1.605 | 25.34837 |
| W | 4.63 | 6.62 | 1 | 1.538 | 29.91565 |
| Re | 3.96 | 7.84 | 1 | 1.6 | 34.23337 |
| Os | 5.14 | 7.26 | 1 | 1.7 | 39.06632 |
| Ir | 5 | 8 | 1 | 1.866 | 43.69259 |

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|---|---|---|---|---|---|
| Pt | 4.79 | 8.86 | 1 | 1.557 | 51.08672 |
| Au | 4.894 | 5.172 | 1 | 1.618 | 57.25236 |
| Hg | 6.27 | 8.32 | 1 | 1.6 | 66.14815 |
| Tl | 3.2 | 5.8 | 1 | 1.53 | 43.69259 |
| Pb | 3.9 | 7.06 | 1 | 1.444 | 47.5736 |
| Bi | 4.53181 | 7.32783 | 1 | 1.514 | 44.87347 |
| Po | 4.42943 | 8.40996 | 1 | 1.48 | 48.8329 |
| At | 4.53674 | 8.99576 | 1 | 1.47 | 55.34395 |
| Rn | 5.37 | 10.74 | 1 | 2.2 | 62.65353 |
| Fr | 2 | 4 | 1 | 2.3 | 6.83259 |
| Ra | 2.843 | 4.868 | 1 | 2.2 | 8.67007 |
| Ac | 2.835 | 5.67 | 1 | 2.108 | 10.34466 |
| Th | 3.175 | 5.81 | 1 | 2.018 | 10.34466 |
| Pa | 2.985 | 5.81 | 1 | 1.8 | 13.07337 |
| U | 3.341 | 5.706 | 1 | 1.713 | 13.33589 |
| Np | 3.549 | 5.434 | 1 | 1.8 | 13.38967 |

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|---|---|---|---|---|---|
| Pu | 3.243 | 5.638 | 1 | 1.84 | 13.55362 |
| Am | 2.9895 | 6.007 | 1 | 1.942 | 14.25166 |
| Cm | 2.8315 | 6.379 | 1 | 1.9 | 14.43755 |
| Bk | 3.1935 | 6.071 | 1 | 1.9 | 14.62836 |
| Cf | 3.197 | 6.202 | 1 | 1.9 | 16.19823 |
| Es | 3.333 | 6.178 | 1 | 1.9 | 16.85603 |
| Fm | 3.4 | 6.2 | 1 | 1.9 | 13.95226 |
| Md | 3.47 | 6.22 | 1 | 1.9 | 18.24526 |
| No | 3.475 | 6.35 | 1 | 1.9 | 20.24779 |
| Lr | 3.5 | 6.4 | 1 | 1.9 | 0 |

**2. Electrostatic Interaction Energy Curves**

Figure S1: A comparison between QM (LACVP**++[1] or ERMLER**++[2] and B3LYP[3]) with PQEq and PQEq2 via the electrostatic interaction dipole energies. A subfigure is depicted for each plot to describe the direction of the dipole scan.