

SUPPORTING INFORMATION:

**Highly Transferable Atomistic Machine-Learning Potentials from Curated and Compact Datasets Across the Periodic Table**

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**Table of Contents**

|   |    |
|---|----|
| Table S1. The total number of configurations included in each iteration of DNP training for each element.....   | 2  |
| Table S2. Comparison of DNP and DFT-derived material properties. ....   | 3  |
| Table S3. Isolated atom DFT $E_{\text{ISO, DFT}}$ (eV) in a 10x10x10 Å box. ....  | 6  |
| Table S4. Comparison of DNP and DFT Vacancy Energies $E_{\text{V, DNP/DFT}}$ (eV) and per atom Volumes $V_{\text{DNP/DFT}}$ (Å <sup>3</sup> /atom). ....  | 7  |
| Table S5. Comparison of DNP and DFT Interstitial Energies $E_{\text{INT, DNP/DFT}}$ (eV) and per atom Volumes $V_{\text{DNP/DFT}}$ (Å <sup>3</sup> /atom). ....   | 8  |
| Table S6. DNP and DFT Elastic Constants (GPa) for ground-state lattices. ....   | 12 |
| Table S7. Additional Elastic Constants (GPa) for Trained Non-Groundstate Structures. ....   | 15 |
| Table S8. DNP and DFT Phases <i>Not</i> Explicitly included in the Training Dataset. ....   | 28 |
| Table S9. Comparison of DNP and DFT Vacancy Energies $E_{\text{V, DNP/DFT}}$ (eV) and per atom Volumes $V_{\text{DNP/DFT}}$ (Å <sup>3</sup> /atom) <i>Not</i> Explicitly included in the Training Dataset. .... | 30 |
| Table S10. Surface Energies Calculated by DNP and DFT (mJ/m <sup>2</sup> ). ....  | 32 |
| REFERENCES.....   | 33 |

**Table S1.** The total number of configurations included in each iteration of DNP training for each element.

| <b>Element</b> | <b>Configurations</b> | <b>Atoms</b>       | <b>Average</b>   | <b>Max Iteration</b> |
|----------------|-----------------------|--------------------|------------------|----------------------|
| Ag             | 3724                  | 103948             | 27.9             | 2                    |
| Al             | 3122                  | 110250             | 35.3             | 3                    |
| Au             | 4104                  | 102619             | 25.0             | 2                    |
| Cu             | 2955                  | 86148              | 29.2             | 3                    |
| Co             | 3553                  | 72162              | 20.3             | 2                    |
| Ge             | 3317                  | 235332             | 70.9             | 1                    |
| I              | 5996                  | 150244             | 24.6             | 3                    |
| Kr             | 2956                  | 86140              | 29.1             | 2                    |
| Li             | 2533                  | 93661              | 37.0             | 3                    |
| Ni             | 3891                  | 77015              | 19.8             | 3                    |
| Nb             | 3188                  | 55084              | 17.3             | 3                    |
| Mg             | 3024                  | 58578              | 19.4             | 1                    |
| Mo             | 3638                  | 65946              | 18.1             | 2                    |
| Os             | 4820                  | 118352             | 24.6             | 3                    |
| Pb             | 5269                  | 118012             | 22.4             | 3                    |
| Pd             | 2348                  | 102264             | 43.6             | 2                    |
| Pt             | 2572                  | 61633              | 24.0             | 3                    |
| Re             | 5330                  | 111190             | 20.9             | 2                    |
| Sb             | 4599                  | 108666             | 23.6             | 2                    |
| Sr             | 4496                  | 65698              | 14.6             | 2                    |
| Ti             | 5160                  | 123919             | 24.0             | 2                    |
| Zn             | 3265                  | 86960              | 26.6             | 1                    |
| Zr             | 4754                  | 80742              | 17.0             | 3                    |
| <b>Total</b>   | <b>3857±1032</b>      | <b>98894±38250</b> | <b>26.7±11.8</b> | <b>2±1</b>           |

**Table S2.** Comparison of DNP and DFT-derived material properties.

| Element | Structure ID                    | Crystal System | $E_{\text{coh, DNP}}$ | s.d   | $E_{\text{coh, DFT}}$ | $V_{\text{DNP}}$ | s.d.  | $V_{\text{DFT}}$ | $E_{\text{coh Error}}$ | $V_{\text{DNP Error}}$ |
|---------|---------------------------------|----------------|-----------------------|-------|-----------------------|------------------|-------|------------------|------------------------|------------------------|
| Ag      | MP-989737                       | rhomb          | -2.667                | 0.004 | -2.669                | 17.715           | 0.022 | 18.051           | 0%                     | 2%                     |
| Ag      | MP-124                          | fcc            | -2.668                | 0.004 | -2.666                | 17.611           | 0.026 | 17.747           | 0%                     | 1%                     |
| Ag      | MP-8566                         | dhcp           | -2.666                | 0.004 | -2.661                | 17.691           | 0.014 | 17.772           | 0%                     | 0%                     |
| Ag      | MP-10597                        | hcp            | -2.665                | 0.005 | -2.671                | 17.754           | 0.039 | 17.758           | 0%                     | 0%                     |
| Ag      | ND-e18KAHKA9NeQjf48uVhl3OmTw2An | ortho          | -2.599                | 0.006 | -2.556                | 18.234           | 0.073 | 19.300           | 2%                     | 6%                     |
| Al      | MP-134                          | fcc            | -3.679                | 0.005 | -3.672                | 16.530           | 0.043 | 16.514           | 0%                     | 0%                     |
| Al      | MP-1183144                      | dhcp           | -3.672                | 0.006 | -3.673                | 16.536           | 0.036 | 16.562           | 0%                     | 0%                     |
| Al      | MP-998860                       | bcc            | -3.606                | 0.008 | -3.568                | 16.400           | 0.056 | 16.978           | 1%                     | 3%                     |
| Al      | MP-1239196                      | tetrag         | -3.291                | 0.01  | -3.375                | 24.045           | 0.063 | 23.924           | 2%                     | 1%                     |
| Al      | sc                              | sc             | -3.405                | 0.014 | -3.304                | 19.765           | 0.369 | 20.084           | 3%                     | 2%                     |
| Au      | MP-81                           | fcc            | -3.186                | 0.008 | -3.164                | 17.667           | 0.178 | 17.947           | 1%                     | 2%                     |
| Au      | MP-1008634                      | hcp            | -3.185                | 0.008 | -3.177                | 17.667           | 0.183 | 17.931           | 0%                     | 1%                     |
| Au      | ND-Vm5tz1VwY8ikjDNa-7trkwSIVnb6 | bcc            | -3.127                | 0.044 | -3.156                | 18.532           | 0.768 | 17.156           | 1%                     | 8%                     |
| Au      | ND-j9Rw6C2osMGGmW84YS-gThlwm-YL | tetrag         | -3.188                | 0.001 | -3.178                | 17.649           | 0.154 | 17.061           | 0%                     | 3%                     |
| Au      | sc                              | sc             | -3.183                | 0.008 | -3.170                | 17.682           | 0.189 | 17.900           | 0%                     | 1%                     |
| Co      | MP-54                           | hcp            | -6.178                | 0.004 | -5.978                | 10.138           | 0.024 | 10.268           | 3%                     | 1%                     |
| Co      | MP-102                          | fcc            | -6.168                | 0.017 | -5.988                | 10.564           | 0.42  | 10.841           | 3%                     | 3%                     |
| Co      | MP-1271679                      | trig           | -6.178                | 0.004 | -5.980                | 10.138           | 0.029 | 10.267           | 3%                     | 1%                     |
| Co      | MP-1193227                      | tetrag         | -6.011                | 0.009 | -5.778                | 11.173           | 0.093 | 10.718           | 4%                     | 4%                     |
| Co      | sc                              | sc             | -5.536                | 0.031 | -5.165                | 12.715           | 0.13  | 11.802           | 6%                     | 8%                     |
| Cu      | MP-30                           | fcc            | -3.660                | 0.003 | -3.678                | 11.928           | 0.017 | 11.929           | 0%                     | 0%                     |
| Cu      | MP-989695                       | dhcp           | -3.661                | 0.003 | -3.674                | 11.918           | 0.028 | 11.947           | 0%                     | 0%                     |
| Cu      | MP-1010136                      | tetrag         | -3.628                | 0.003 | -3.646                | 11.984           | 0.055 | 12.003           | 0%                     | 0%                     |
| Cu      | MP-998890                       | bcc            | -3.628                | 0.004 | -3.645                | 11.974           | 0.055 | 11.985           | 0%                     | 0%                     |
| Cu      | MP-1120774                      | trig           | -3.505                | 0.002 | -3.521                | 22.371           | 0.253 | 22.572           | 0%                     | 1%                     |
| Ge      | MP-32                           | diamond        | -4.255                | 0.001 | -4.393                | 23.492           | 0.154 | 23.757           | 3%                     | 1%                     |
| Ge      | MP-1091415                      | hcp            | -4.268                | 0.003 | -4.387                | 23.682           | 0.04  | 23.704           | 3%                     | 0%                     |
| Ge      | MP-1080106                      | cubic          | -4.229                | 0.005 | -4.254                | 21.470           | 0.76  | 21.877           | 1%                     | 2%                     |
| Ge      | MP-137                          | tertag         | -4.200                | 0.003 | -4.250                | 21.193           | 0.258 | 21.315           | 1%                     | 1%                     |
| Ge      | MP-78                           | tetrag         | -4.175                | 0.002 | -4.162                | 19.146           | 0.149 | 19.232           | 0%                     | 0%                     |
| I       | MP-23153                        | ortho          | -1.335                | 0.082 | -1.440                | 54.085           | 2.26  | 51.215           | 7%                     | 6%                     |
| I       | MP-639751                       | ortho          | -1.375                | 0.019 | -1.393                | 47.344           | 0.165 | 48.996           | 1%                     | 3%                     |
| I       | MP-1180981                      | ortho          | -1.255                | 0.009 | -1.322                | 46.214           | 0.532 | 47.834           | 5%                     | 3%                     |
| I       | MP-601148                       | tetrag         | -1.254                | 0.009 | -1.340                | 46.130           | 0.53  | 47.570           | 6%                     | 3%                     |
| I       | MP-684663                       | bcc            | -1.100                | 0.029 | -0.978                | 36.014           | 0.463 | 35.879           | 12%                    | 0%                     |
| Kr      | MP-612118                       | fcc            | -0.085                | 0.082 | -0.042                | 66.025           | 0.93  | 61.625           | 113%                   | 7%                     |
| Kr      | MP-975590                       | rhomb          | -0.085                | 0.061 | -0.045                | 62.261           | 0.904 | 65.652           | 98%                    | 5%                     |
| Kr      | MP-976347                       | dhcp           | -0.097                | 0.08  | -0.045                | 62.188           | 1.961 | 65.753           | 127%                   | 5%                     |
| Kr      | MP-567365                       | hcp            | -0.097                | 0.081 | -0.045                | 62.176           | 1.952 | 65.673           | 127%                   | 5%                     |
| Kr      | MP-974400                       | bcc            | -0.057                | 0.033 | -0.045                | 66.053           | 0.933 | 65.770           | 29%                    | 0%                     |
| Li      | MP-1018134                      | rhomb          | -1.856                | 0.002 | -1.857                | 20.215           | 0.058 | 20.293           | 0%                     | 0%                     |

|    |                                     |         |         |       |        |        |       |        |    |    |
|----|-------------------------------------|---------|---------|-------|--------|--------|-------|--------|----|----|
| Li | MP-976411                           | dhcp    | -1.858  | 0.002 | -1.856 | 20.134 | 0.041 | 20.302 | 0% | 1% |
| Li | MP-51                               | fcc     | -1.859  | 0.002 | -1.853 | 19.755 | 0.462 | 20.370 | 0% | 3% |
| Li | MP-135                              | bcc     | -1.859  | 0.001 | -1.851 | 20.401 | 0.072 | 20.386 | 0% | 0% |
| Li | MP-1063005                          | hex     | -1.858  | 0.001 | -1.859 | 20.404 | 0.069 | 20.306 | 0% | 0% |
| Mo | 0_mp-129                            | bcc     | -10.545 | 0.045 | 10.617 | 15.643 | 0.164 | 15.762 | 1% | 1% |
| Mo | 3_mp-8637                           | fcc     | -10.275 | 0.006 | 10.181 | 16.154 | 0.372 | 15.996 | 1% | 1% |
| Mo | 4_mp-1066523                        | dhcp    | -10.266 | 0.001 | 10.188 | 16.128 | 0.274 | 16.062 | 1% | 0% |
| Mo | 6_mp-1056004                        | hex     | -9.847  | 0.029 | -9.756 | 16.502 | 0.432 | 16.733 | 1% | 1% |
| Mo | sc                                  | sc      | -9.608  | 0.014 | -9.461 | 17.683 | 0.644 | 17.542 | 2% | 1% |
| Mg | MP-1056702                          | fcc     | -1.510  | 0.002 | -1.498 | 22.717 | 0.172 | 23.134 | 1% | 2% |
| Mg | MP-1094122                          | rhomb   | -1.508  | 0.002 | -1.510 | 22.635 | 0.164 | 22.997 | 0% | 2% |
| Mg | MP-153                              | hcp     | -1.511  | 0.003 | -1.514 | 22.564 | 0.154 | 22.889 | 0% | 1% |
| Mg | MP-973364                           | dhcp    | -1.376  | 0.001 | -1.513 | 23.899 | 0.197 | 22.922 | 9% | 4% |
| Mg | MP-1247180                          | ortho   | -1.511  | 0.003 | -1.511 | 22.582 | 0.16  | 22.881 | 0% | 1% |
| Nb | MP-75                               | Bcc     | -9.507  | 0.081 | -9.473 | 18.343 | 0.371 | 18.104 | 0% | 1% |
| Nb | MP-109412                           | fcc     | -9.279  | 0.064 | -9.307 | 18.616 | 0.147 | 18.576 | 0% | 0% |
| Nb | MP-8636                             | hcp     | -9.506  | 0.081 | -9.483 | 18.344 | 0.37  | 18.030 | 0% | 2% |
| Nb | ND-InngSFTjbQPoKX5<br>ZtDChEkeekVzo | diamond | -9.507  | 0.081 | -9.494 | 18.341 | 0.372 | 17.186 | 0% | 7% |
| Nb | sc                                  | sc      | -8.492  | 0.119 | -8.524 | 20.949 | 1.239 | 19.956 | 0% | 5% |
| Ni | MP-23                               | fcc     | -4.871  | 0.005 | -4.837 | 10.854 | 0.062 | 10.791 | 1% | 1% |
| Ni | MP-10257                            | hcp     | -4.864  | 0.009 | -4.814 | 10.820 | 0.021 | 10.822 | 1% | 0% |
| Ni | MP-1008728                          | bcc     | -4.797  | 0.009 | -4.785 | 10.766 | 0.09  | 10.844 | 0% | 1% |
| Ni | MP-1014111                          | trig    | -4.864  | 0.009 | -4.814 | 10.820 | 0.021 | 10.822 | 1% | 0% |
| Ni | MP-1094136                          | hex     | -4.871  | 0.004 | -4.838 | 10.852 | 0.064 | 10.788 | 1% | 1% |
| Os | MP-49                               | hcp     | -10.059 | 0.006 | 10.312 | 14.167 | 0.249 | 14.269 | 2% | 1% |
| Os | MP-8643                             | fcc     | -10.098 | 0.005 | 10.172 | 14.189 | 0.263 | 14.326 | 1% | 1% |
| Os | bcc                                 | bcc     | -9.974  | 0.024 | 10.087 | 14.500 | 0.031 | 14.788 | 1% | 2% |
| Os | ND-w3arEIPCdTvj6s3-<br>QgGt6YXTAhGK | rhomb   | -9.813  | 0.025 | -9.806 | 19.913 | 0.502 | 21.137 | 0% | 6% |
| Os | ND-5FQY1cKaxcYqrPY<br>N2iyvrtKPIGeh | tertag  | -10.098 | 0.005 | 10.169 | 19.188 | 0.261 | 20.521 | 1% | 6% |
| Pb | MP-20483                            | fcc     | -3.449  | 0.01  | -3.469 | 31.375 | 0.192 | 31.828 | 1% | 1% |
| Pb | MP-1186444                          | dhcp    | -3.451  | 0.009 | -3.467 | 31.365 | 0.16  | 31.609 | 0% | 1% |
| Pb | MP-22692                            | bcc     | -3.425  | 0.001 | -3.422 | 32.562 | 0.816 | 32.001 | 0% | 2% |
| Pb | MP-1057273                          | rhomb   | -3.419  | 0.007 | -3.408 | 32.076 | 0.317 | 33.777 | 0% | 5% |
| Pb | MP-1247117                          | diamond | -3.005  | 0.021 | -3.201 | 45.035 | 0.629 | 43.657 | 6% | 3% |
| Pd | MP-2                                | fcc     | -3.803  | 0.011 | -3.775 | 15.307 | 0.108 | 15.282 | 1% | 0% |

|    |                                  |          |         |       |        |        |       |        |    |     |
|----|----------------------------------|----------|---------|-------|--------|--------|-------|--------|----|-----|
| Pd | MP-1186427                       | hcp      | -3.791  | 0.013 | -3.764 | 15.290 | 0.113 | 15.295 | 1% | 0%  |
| Pd | ND-AzTtp                         | tetrag   | -3.803  | 0.011 | -3.774 | 15.309 | 0.108 | 15.248 | 1% | 0%  |
| Pd | ND-DUqr43                        | rhomb    | -3.803  | 0.012 | -3.786 | 15.309 | 0.11  | 14.520 | 0% | 5%  |
| Pd | diamond                          | diamond  | -2.966  | 0.615 | -2.646 | 21.352 | 3.944 | 24.304 | 8% | 12% |
| Pt | MP-126                           | fcc      | -5.894  | 0.032 | -5.926 | 15.619 | 0.116 | 15.603 | 1% | 0%  |
| Pt | ND-cGAS2LRJaQh-bvTdqx4mGBiHwcBF  | hcp      | -5.804  | 0.022 | -5.912 | 15.943 | 0.048 | 15.783 | 2% | 1%  |
| Pt | ND-5COO2H3XeXwKr q0BOxP3IzWgNkUY | hcp      | -5.871  | 0.027 | -5.863 | 15.665 | 0.108 | 14.959 | 0% | 5%  |
| Pt | ND-C9BvrCuSR5pUZ9Ec1SBqSvCjV04O  | bcc      | -5.827  | 0.051 | -5.804 | 15.917 | 0.229 | 15.071 | 0% | 6%  |
| Pt | diamond                          | diamond  | -5.150  | 0.379 | -4.849 | 21.564 | 3.745 | 23.973 | 6% | 10% |
| Re | MP-8                             | hcp      | -10.667 | 0.012 | 10.826 | 14.876 | 0.023 | 14.931 | 1% | 0%  |
| Re | MP-1186901                       | dhcp     | -10.507 | 0.064 | 10.758 | 24.813 | 0.093 | 23.644 | 2% | 5%  |
| Re | MP-975065                        | trigonal | -10.670 | 0.014 | 10.807 | 14.866 | 0.027 | 14.944 | 1% | 1%  |
| Re | MP-8642                          | fcc      | -10.677 | 0.016 | 10.758 | 14.852 | 0.041 | 14.980 | 1% | 1%  |
| Re | sc                               | sc       | -9.728  | 0.042 | -9.460 | 17.062 | 0.324 | 17.123 | 2% | 0%  |
| Sb | MP-104                           | Rhomb    | -3.914  | 0.001 | -4.011 | 31.684 | 0.113 | 31.783 | 2% | 0%  |
| Sb | MP-1179605                       | ortho    | -3.893  | 0.005 | -3.947 | 30.027 | 0.307 | 30.042 | 1% | 0%  |
| Sb | MP-10630                         | fcc      | -3.696  | 0.014 | -3.689 | 27.687 | 0.135 | 27.334 | 0% | 1%  |
| Sb | MP-133                           | sc       | -3.895  | 0.005 | -3.956 | 29.965 | 0.329 | 29.919 | 1% | 0%  |
| Sb | MP-7761                          | bcc      | -3.794  | 0.013 | -3.765 | 27.115 | 0.653 | 27.272 | 1% | 1%  |
| Sr | MP-1187073                       | trig     | -1.618  | 0.004 | -1.615 | 55.771 | 0.555 | 55.004 | 0% | 1%  |
| Sr | MP-139                           | hcp      | -1.619  | 0.003 | -1.612 | 55.763 | 0.563 | 55.018 | 0% | 1%  |
| Sr | MP-76                            | fcc      | -1.618  | 0.004 | -1.615 | 55.766 | 0.558 | 54.695 | 0% | 2%  |
| Sr | MP-95                            | bcc      | -1.612  | 0.008 | -1.607 | 55.293 | 0.239 | 53.420 | 0% | 4%  |
| Sr | MP-1179325                       | tetrag   | -1.207  | 0.016 | -1.216 | 59.843 | 0.459 | 55.253 | 1% | 8%  |
| Ti | MP-72                            | Hex      | -6.125  | 0.015 | -6.209 | 17.035 | 0.085 | 16.843 | 1% | 1%  |
| Ti | MP-46                            | hcp      | -6.179  | 0.005 | -6.195 | 16.896 | 0.062 | 17.119 | 0% | 1%  |
| Ti | MP-6985                          | fcc      | -6.209  | 0.005 | -6.137 | 16.929 | 0.038 | 17.133 | 1% | 1%  |
| Ti | MP-73                            | bcc      | -6.111  | 0.004 | -6.093 | 17.085 | 0.109 | 16.955 | 0% | 1%  |
| Ti | sc                               | sc       | -5.552  | 0.049 | -5.386 | 18.185 | 0.241 | 18.123 | 2% | 0%  |
| Zn | MP-79                            | hcp      | -1.078  | 0.001 | -1.104 | 15.148 | 0.091 | 15.029 | 2% | 1%  |
| Zn | MP-1187812                       | rhomb    | -1.084  | 0.001 | -1.095 | 15.064 | 0.105 | 15.018 | 1% | 0%  |
| Zn | ND-hxNPwQaO0Pg_2-2v8T_6JeSoclea  | fcc      | -1.097  | 0.002 | -1.084 | 15.053 | 0.043 | 15.806 | 1% | 5%  |
| Zn | ND-wLmvfrkizZXcCSH N-rhL9n5uqaft | bcc      | -1.034  | 0.009 | -1.021 | 15.051 | 0.224 | 14.551 | 1% | 3%  |

|    |            |         |        |       |        |        |       |        |     |    |
|----|------------|---------|--------|-------|--------|--------|-------|--------|-----|----|
| Zn | diamond    | diamond | -0.699 | 0.23  | -0.627 | 22.408 | 1.197 | 24.516 | 11% | 9% |
| Zr | MP-131     | hcp     | -7.188 | 0.026 | -7.114 | 23.185 | 0.074 | 23.150 | 1%  | 0% |
| Zr | MP-1077723 | ortho   | -7.150 | 0.022 | -7.142 | 23.158 | 0.078 | 23.332 | 0%  | 1% |
| Zr | MP-8635    | fcc     | -7.188 | 0.026 | -7.127 | 23.189 | 0.074 | 23.178 | 1%  | 0% |
| Zr | MP-1056376 | hex     | -6.718 | 0.014 | -6.790 | 24.188 | 0.35  | 23.789 | 1%  | 2% |
| Zr | MP-1178608 | hex     | -7.130 | 0.016 | -7.092 | 23.158 | 0.142 | 22.864 | 0%  | 1% |

For the crystal phases bcc = body centered cubic, diamond = diamond cubic, dhcp = double hexagonal close packed, fcc = face center cubic, hex = hexagonal, hcp = hexagonal close packed, ortho = orthorhombic, rhomb = rhombohedral, sc = simple cubic, tetrag = tetragonal, trig = trigonal.

**Table S3.** Isolated atom DFT  $E_{\text{ISO, DFT}}$  (eV) in a 10x10x10 Å box.

| Element | $E_{\text{ISO, DFT}}$ |
|---------|-----------------------|
| Al      | -0.0712               |
| Ag      | -0.0520               |
| Au      | -0.0502               |
| Cu      | -0.0519               |
| Co      | -0.8416               |
| Ge      | -0.1232               |
| I       | -0.0773               |
| Kr      | 0.0035                |
| Li      | -0.0443               |
| Nb      | -0.7295               |
| Ni      | -0.5739               |
| Mg      | 0.0081                |
| Mo      | -0.3075               |
| Os      | -0.9355               |
| Pb      | -0.1089               |
| Pd      | -1.4309               |
| Pt      | -0.1787               |
| Re      | -1.6024               |
| Sb      | -0.1347               |
| Sr      | -0.0218               |
| Ti      | -1.5673               |
| Zr      | -1.3615               |
| Zn      | -0.0018               |

These reference energies were used to calculate the  $E_{\text{coh}}$

**Table S4.** Comparison of DNP and DFT Vacancy Energies  $E_{v, \text{DNP/DFT}}$  (eV) and per atom Volumes  $V_{\text{DNP/DFT}}$  ( $\text{\AA}^3/\text{atom}$ ).

| Element | MPDB-ID#   | $V_{\text{DNP}}$ | s.d.<br>$V_{\text{DNP}}$ | $V_{\text{DFT}}$ | atoms | $E_{v, \text{DNP}}$ | s.d.<br>$E_{v, \text{DNP}}$ | $E_{v, \text{DFT}}$ | $E_v$ Error<br>(%) |
|---------|------------|------------------|--------------------------|------------------|-------|---------------------|-----------------------------|---------------------|--------------------|
| Ag      | MP-989737  | 18.25            | 0.034                    | 18.341           | 23    | 0.772               | 0.034                       | 0.9                 | 17                 |
| Al      | MP-134     | 16.51            | 0.281                    | 16.855           | 31    | 0.61                | 0.045                       | 0.5                 | 28                 |
| Au      | MP-81      | 19.4             | 0.167                    | 20.497           | 7     | 0.659               | 0.045                       | 0.4                 | 60                 |
| Co      | MP-54      | 11.04            | 0.022                    | 10.678           | 15    | 1.78                | 0.136                       | 1.5                 | 15                 |
| Cu      | MP-30      | 12.15            | 0.006                    | 12.179           | 31    | 1.071               | 0.038                       | 1.1                 | 6                  |
| Ge      | MP-32      | 23.18            | 0.338                    | 24.503           | 15    | 1.349               | 0.068                       | 2.1                 | 35                 |
| I       | MP-639751  | 47.45            | 0.303                    | 48.297           | 15    | 1.076               | 0.178                       | 0.7                 | 48                 |
| Kr      | MP-612118  | 67.358           | 1.034                    | 69.274           | 7     | 0.08                | 0.02                        | 0                   | 700                |
| Li      | MP-135     | 21.37            | 0.12                     | 21.162           | 15    | 0.603               | 0.025                       | 0.5                 | 27                 |
| Mg      | MP-153     | 23.75            | 0.151                    | 23.935           | 15    | 0.738               | 0.021                       | 0.7                 | 1                  |
| Mo      | MP-129     | 16.61            | 0.084                    | 16.4             | 15    | 3.149               | 0.388                       | 3                   | 5                  |
| Nb      | MP-75      | 19.09            | 0.204                    | 18.803           | 15    | 3.134               | 0.106                       | 2.7                 | 15                 |
| Ni      | MP-23      | 11.16            | 0.078                    | 11.002           | 31    | 1.352               | 0.003                       | 1.4                 | 3                  |
| Os      | MP-49      | 14.41            | 0.037                    | 14.918           | 15    | 2.597               | 0.347                       | 3.3                 | 21                 |
| Pb      | MP-20483   | 34.27            | 0.504                    | 34.31            | 7     | 0.395               | 0.133                       | 0.5                 | 21                 |
| Pd      | MP-2       | 15.72            | 0.058                    | 15.564           | 31    | 1.037               | 0.024                       | 0.9                 | 20                 |
| Pt      | MP-126     | 15.92            | 0.082                    | 15.88            | 31    | 1.136               | 0.131                       | 1.1                 | 8                  |
| Re      | MP-8       | 15.28            | 0.015                    | 15.606           | 15    | 2.925               | 0.143                       | 3.4                 | 14                 |
| Sb      | MP-104     | 31.94            | 0.16                     | 31.977           | 47    | 1.053               | 0.1                         | 1.7                 | 36                 |
| Sr      | MP-76      | 56.75            | 0.18                     | 55.913           | 31    | 0.854               | 0.04                        | 1.1                 | 21                 |
| Ti      | MP-46      | 17.49            | 0.056                    | 18.514           | 15    | 1.964               | 0.093                       | 2.1                 | 9                  |
| Zn      | MP-1187812 | 15.25            | 0.067                    | 15.179           | 47    | 0.336               | 0.023                       | 0.2                 | 49                 |
| Zr      | MP-131     | 24.03            | 0.183                    | 24.243           | 15    | 2.124               | 0.123                       | 1.4                 | 48                 |

**Table S5.** Comparison of DNP and DFT Interstitial Energies  $E_{\text{INT, DNP/DFT}}$  (eV) and per atom Volumes  $V_{\text{DNP/DFT}}$  ( $\text{\AA}^3/\text{atom}$ ).

| Element | MPDB-ID#           | $V_{\text{DNP}}$ | s.d.<br>$V_{\text{DNP}}$ | $V_{\text{DFT}}$ | atom | $E_{\text{INT, DNP}}$ | s.d.<br>$E_{\text{INT, DNP}}$ | $E_{\text{INT, DFT}}$ | $E_v$ Error (%) |
|---------|--------------------|------------------|--------------------------|------------------|------|-----------------------|-------------------------------|-----------------------|-----------------|
| Ag      | MP-124_crowdion    | 18.264           | 0.017                    | 18.295           | 33   | 2.394                 | 0.034                         | 2.411                 | 1%              |
| Ag      | MP-124_db100       | 18.308           | 0.055                    | 18.3             | 33   | 2.484                 | 0.111                         | 2.572                 | 3%              |
| Ag      | MP-124_db110       | 18.436           | 0.089                    | 18.374           | 33   | 2.94                  | 0.036                         | 3.063                 | 4%              |
| Ag      | MP-124_db111       | 18.38            | 0.009                    | 18.403           | 33   | 3.001                 | 0.421                         | 3.404                 | 12%             |
| Ag      | MP-124_Oh          | 18.264           | 0.017                    | 18.295           | 33   | 2.394                 | 0.034                         | 2.411                 | 1%              |
| Ag      | MP-124_Td          | 18.536           | 0.166                    | 18.447           | 33   | 3.451                 | 0.096                         | 3.589                 | 4%              |
| Al      | MP-134_crowdion    | 17.139           | 0.352                    | 17.107           | 33   | 2.288                 | 0.005                         | 2.374                 | 4%              |
| Al      | MP-134_db100       | 16.756           | 0.562                    | 17.073           | 33   | 2.379                 | 0.09                          | 2.402                 | 1%              |
| Al      | MP-134_db110       | 17.91            | 0.767                    | 17.163           | 33   | 2.542                 | 0.035                         | 2.471                 | 3%              |
| Al      | MP-134_db111       | 17.8             | 0.711                    | 17.127           | 33   | 2.307                 | 0.045                         | 2.841                 | 19%             |
| Al      | MP-134_Oh          | 17.127           | 0.352                    | 17.107           | 33   | 2.288                 | 0.005                         | 2.374                 | 4%              |
| Al      | MP-134_Td          | 17.781           | 0.89                     | 17.232           | 33   | 2.95                  | 0.569                         | 3.222                 | 8%              |
| Au      | MP-81_crowdion     | 18.474           | 0.043                    | 17.578           | 33   | 2.479                 | 0.114                         | 2.095                 | 18%             |
| Au      | MP-81_db100        | 18.483           | 0.043                    | 18.523           | 33   | 2.789                 | 0.138                         | 2.472                 | 13%             |
| Au      | MP-81_db110        | 18.271           | 0.388                    | 18.612           | 33   | 2.086                 | 0.858                         | 2.51                  | 17%             |
| Au      | MP-81_db111        | 18.676           | 0.036                    | 17.578           | 33   | 3.939                 | 0.165                         | 2.784                 | 41%             |
| Au      | MP-81_Oh           | 18.474           | 0.043                    | 18.495           | 33   | 2.479                 | 0.114                         | 2.095                 | 18%             |
| Au      | MP-81_Td           | 18.477           | 0.043                    | 19.212           | 33   | 2.507                 | 0.117                         | 2.777                 | 10%             |
| Co      | MP-54_crowdion     | 10.959           | 0.05                     | 10.607           | 17   | 2.112                 | 0.071                         | 2.076                 | 2%              |
| Co      | MP-54_dbP          | 11.015           | 0.027                    | 10.61            | 17   | 2.308                 | 0.105                         | 2.411                 | 4%              |
| Co      | MP-54_dbP          | 10.96            | 0.048                    | 10.603           | 17   | 2.114                 | 0.071                         | 2.163                 | 2%              |
| Co      | MP-54_db           | 11.334           | 0.019                    | 10.264           | 17   | 3.858                 | 0.101                         | 4.199                 | 8%              |
| Co      | MP-54_OhB          | 11.043           | 0.022                    | 10.83            | 17   | 2.628                 | 0.07                          | 2.077                 | 27%             |
| Co      | MP-54_Oh           | 11.282           | 0.036                    | 10.705           | 17   | 3.785                 | 0.207                         | 4.549                 | 17%             |
| Co      | MP-54_TdB          | 11.628           | 0.042                    | 10.264           | 17   | 4.787                 | 0.252                         | 4.199                 | 14%             |
| Co      | MP-54_Td           | 11.628           | 0.042                    | 10.264           | 17   | 4.787                 | 0.252                         | 4.199                 | 14%             |
| Cu      | MP-30_crowdion     | 12.227           | 0.025                    | 11.452           | 33   | 2.761                 | 0.036                         | 2.816                 | 2%              |
| Cu      | MP-30_db100        | 12.22            | 0.025                    | 11.452           | 33   | 2.846                 | 0.005                         | 2.895                 | 2%              |
| Cu      | MP-30_db110        | 12.274           | 0.03                     | 12.326           | 33   | 3.229                 | 0.217                         | 3.547                 | 9%              |
| Cu      | MP-30_db111        | 12.304           | 0.04                     | 11.452           | 33   | 2.773                 | 0.016                         | 2.899                 | 4%              |
| Cu      | MP-30_Oh           | 12.23            | 0.024                    | 12.26            | 33   | 2.774                 | 0.036                         | 2.895                 | 4%              |
| Cu      | MP-30_Td           | 12.227           | 0.025                    | 11.452           | 33   | 2.761                 | 0.036                         | 2.899                 | 5%              |
| Ge      | MP-32_db100        | 23.567           | 0.111                    | 23.905           | 65   | 2.501                 | 0.251                         | 2.963                 | 16%             |
| Ge      | MP-32_db110        | 23.568           | 0.11                     | 23.907           | 65   | 2.501                 | 0.251                         | 2.963                 | 16%             |
| Ge      | MP-32_interOh      | 23.568           | 0.11                     | 23.909           | 65   | 2.501                 | 0.251                         | 2.964                 | 16%             |
| Ge      | MP-32_interTd      | 23.568           | 0.11                     | 23.906           | 65   | 2.501                 | 0.251                         | 2.783                 | 10%             |
| Ge      | MP-32_mirror       | 23.568           | 0.11                     | 23.906           | 65   | 2.501                 | 0.251                         | 2.961                 | 16%             |
| Kr      | MP-612118_crowdion | 292.425          | 117.225                  | 67.669           | 33   | 0.081                 | 0.079                         | 0.003                 | 2600%           |
| Kr      | MP-612118_db100    | 303.834          | 114.136                  | 67.662           | 33   | 0.08                  | 0.07                          | 0.023                 | 248%            |
| Kr      | MP-612118_db110    | 434.458          | 239.204                  | 75.192           | 33   | 0.134                 | 0.1                           | 0.244                 | 45%             |
| Kr      | MP-612118_db111    | 316.528          | 127.171                  | 68.234           | 33   | 0.029                 | 0.037                         | 0.008                 | 263%            |
| Kr      | MP-612118_Oh       | 289.768          | 107.162                  | 68.241           | 33   | 0.014                 | 0.059                         | 0.005                 | 180%            |
| Kr      | MP-612118_Td       | 321.371          | 135.827                  | 68.819           | 33   | 0.041                 | 0.39                          | 0.011                 | 273%            |



|    |                   |        |       |        |    |       |       |       |     |
|----|-------------------|--------|-------|--------|----|-------|-------|-------|-----|
| Li | MP-135_crowdion   | 20.791 | 0.218 | 20.72  | 17 | 0.693 | 0.01  | 0.673 | 3%  |
| Li | MP-135_db100      | 20.66  | 0.15  | 20.781 | 17 | 0.842 | 0.033 | 0.713 | 18% |
| Li | MP-135_db110      | 20.898 | 0.172 | 20.703 | 17 | 0.804 | 0.018 | 0.671 | 20% |
| Li | MP-135_db111      | 20.793 | 0.219 | 20.72  | 17 | 0.693 | 0.009 | 0.673 | 3%  |
| Li | MP-135_Oh         | 20.833 | 0.154 | 20.641 | 17 | 0.735 | 0.02  | 0.595 | 24% |
| Li | MP-135_Td         | 20.587 | 0.07  | 20.618 | 17 | 0.628 | 0.024 | 0.485 | 29% |
| Mg | MP-153_crowdionB  | 23.463 | 0.192 | 23.633 | 17 | 0.832 | 0.01  | 1.026 | 19% |
| Mg | MP-153_crowdionB  | 23.87  | 0.12  | 24.042 | 17 | 1.642 | 0.007 | 1.686 | 3%  |
| Mg | MP-153_crowdion   | 23.45  | 0.235 | 23.532 | 17 | 0.79  | 0.014 | 0.896 | 12% |
| Mg | MP-153_dbP        | 23.497 | 0.22  | 23.665 | 17 | 0.784 | 0.012 | 0.841 | 7%  |
| Mg | MP-153_dbPP       | 23.703 | 0.141 | 24.256 | 17 | 1.407 | 0.041 | 1.62  | 13% |
| Mg | MP-153_dbP        | 23.5   | 0.213 | 23.621 | 17 | 0.781 | 0.01  | 0.776 | 1%  |
| Mg | MP-153_db         | 24.114 | 0.503 | 24.255 | 17 | 1.647 | 0.221 | 1.62  | 2%  |
| Mg | MP-153_OhB        | 23.502 | 0.21  | 23.635 | 17 | 0.78  | 0.01  | 0.773 | 1%  |
| Mg | MP-153_Oh         | 24.392 | 0.26  | 24.344 | 17 | 1.645 | 0.009 | 1.777 | 7%  |
| Mg | MP-153_TdB        | 24.504 | 0.319 | 25.171 | 17 | 2.436 | 0.054 | 3.904 | 38% |
| Mg | MP-153_Td         | 23.703 | 0.141 | 24.255 | 17 | 1.408 | 0.041 | 1.62  | 13% |
| Nb | MP-75_crowdion    | 18.704 | 0.246 | 17.22  | 17 | 5.392 | 0.436 | 3.998 | 35% |
| Nb | MP-75_db100       | 18.833 | 0.157 | 18.755 | 17 | 5.404 | 0.436 | 5.966 | 9%  |
| Nb | MP-75_db110       | 18.773 | 0.198 | 17.22  | 17 | 4.192 | 0.397 | 3.985 | 5%  |
| Nb | MP-75_db111       | 18.699 | 0.231 | 17.22  | 17 | 5.419 | 0.436 | 3.985 | 36% |
| Nb | MP-75_Oh          | 18.655 | 0.263 | 17.22  | 17 | 4.02  | 0.264 | 3.985 | 1%  |
| Nb | MP-75_Td          | 18.822 | 0.239 | 17.22  | 17 | 4.972 | 0.277 | 3.985 | 25% |
| Ni | MP-23_crowdion    | 11.168 | 0.085 | 11.055 | 33 | 3.66  | 0.145 | 3.546 | 3%  |
| Ni | MP-23_db100       | 11.168 | 0.094 | 11.057 | 33 | 3.759 | 0.134 | 3.68  | 2%  |
| Ni | MP-23_db110       | 11.214 | 0.074 | 11.095 | 33 | 4.022 | 0.141 | 4.381 | 8%  |
| Ni | MP-23_db111       | 11.183 | 0.08  | 11.099 | 33 | 3.78  | 0.14  | 4.505 | 16% |
| Ni | MP-23_Oh          | 11.168 | 0.085 | 11.055 | 33 | 3.66  | 0.145 | 3.546 | 3%  |
| Ni | MP-23_Td          | 11.168 | 0.085 | 11.057 | 33 | 3.66  | 0.145 | 3.545 | 3%  |
| Os | MP-49_crowdionB   | 15.472 | 0.323 | 15.273 | 17 | 6.697 | 0.687 | 7.948 | 16% |
| Os | MP-49_crowdionP   | 15.572 | 0.534 | 15.751 | 17 | 6.743 | 0.527 | 7.416 | 9%  |
| Os | MP-49_crowdion    | 15.573 | 0.535 | 15.754 | 17 | 6.746 | 0.526 | 7.423 | 9%  |
| Os | MP-49_dbB         | 15.632 | 0.36  | 15.606 | 17 | 6.293 | 0.579 | 7.515 | 16% |
| Os | MP-49_dbP         | 15.422 | 0.26  | 15.6   | 17 | 7.057 | 0.446 | 7.524 | 6%  |
| Os | MP-49_dbP         | 15.342 | 0.114 | 15.271 | 17 | 7.473 | 0.389 | 7.936 | 6%  |
| Os | MP-49_db          | 15.272 | 0.055 | 15.194 | 17 | 8.423 | 0.539 | 9.424 | 11% |
| Os | MP-49_OhB         | 15.424 | 0.331 | 15.773 | 17 | 6.688 | 0.597 | 7.27  | 8%  |
| Os | MP-49_Oh          | 15.373 | 0.097 | 15.19  | 17 | 9.212 | 0.264 | 9.569 | 4%  |
| Os | MP-49_TdB         | 15.574 | 0.534 | 15.751 | 17 | 7.744 | 0.526 | 7.416 | 4%  |
| Os | MP-49_Td          | 15.253 | 0.063 | 15.554 | 17 | 8.879 | 0.488 | 9.004 | 1%  |
| Pb | MP-20483_crowdion | 32.285 | 0.29  | 32.667 | 33 | 1.257 | 0.075 | 1.975 | 36% |
| Pb | MP-20483_db100    | 32.778 | 0.289 | 32.501 | 33 | 1.398 | 0.148 | 2.026 | 31% |
| Pb | MP-20483_db110    | 32.609 | 0.304 | 32.643 | 33 | 1.449 | 0.206 | 2.042 | 29% |
| Pb | MP-20483_db111    | 32.815 | 0.116 | 32.681 | 33 | 1.363 | 0.287 | 2.235 | 39% |
| Pb | MP-20483_Oh       | 32.285 | 0.29  | 32.666 | 33 | 1.257 | 0.075 | 1.975 | 36% |
| Pb | MP-20483_Td       | 32.386 | 0.26  | 32.873 | 33 | 1.743 | 0.496 | 2.331 | 25% |
| Pd | MP-2_crowdion     | 15.655 | 0.066 | 15.684 | 33 | 3.451 | 0.299 | 3.237 | 7%  |
| Pd | MP-2_db100        | 15.658 | 0.066 | 15.698 | 33 | 3.493 | 0.303 | 3.506 | 0%  |
| Pd | MP-2_db110        | 15.836 | 0.024 | 15.751 | 33 | 3.864 | 0.317 | 4.067 | 5%  |

|    |                 |        |       |        |    |       |       |       |     |
|----|-----------------|--------|-------|--------|----|-------|-------|-------|-----|
| Pd | MP-2_db111      | 15.654 | 0.066 | 15.684 | 33 | 3.453 | 0.298 | 3.247 | 6%  |
| Pd | MP-2_Oh         | 15.654 | 0.067 | 15.684 | 33 | 3.451 | 0.299 | 3.235 | 7%  |
| Pd | MP-2_Td         | 15.655 | 0.066 | 15.779 | 33 | 3.451 | 0.299 | 4.61  | 25% |
| Pt | MP-126_crowdion | 16.1   | 0.071 | 16.061 | 33 | 3.734 | 0.172 | 4.468 | 16% |
| Pt | MP-126_db100    | 16.104 | 0.071 | 16.094 | 33 | 3.763 | 0.169 | 5.305 | 29% |
| Pt | MP-126_db110    | 16.099 | 0.028 | 16.246 | 33 | 4.399 | 0.227 | 5.203 | 15% |
| Pt | MP-126_db111    | 16.102 | 0.071 | 16.228 | 33 | 5.763 | 0.17  | 6.433 | 10% |
| Pt | MP-126_Oh       | 16.1   | 0.071 | 16.061 | 33 | 3.734 | 0.172 | 4.468 | 16% |
| Pt | MP-126_Td       | 16.1   | 0.071 | 16.061 | 33 | 4.734 | 0.172 | 4.468 | 6%  |
| Re | MP-8_crowdionB  | 15.559 | 0.206 | 15.779 | 17 | 4.543 | 0.253 | 5.956 | 24% |
| Re | MP-8_crowdionB  | 15.764 | 0.191 | 16.202 | 17 | 6.198 | 0.353 | 7.091 | 13% |
| Re | MP-8_crowdionP  | 15.541 | 0.207 | 15.78  | 17 | 4.587 | 0.207 | 5.961 | 23% |
| Re | MP-8_crowdion   | 15.552 | 0.202 | 15.782 | 17 | 4.506 | 0.275 | 5.96  | 24% |
| Re | MP-8_dbB        | 15.765 | 0.194 | 16.223 | 17 | 6.197 | 0.353 | 7.091 | 13% |
| Re | MP-8_dbP        | 15.553 | 0.203 | 15.782 | 17 | 4.504 | 0.276 | 5.96  | 24% |
| Re | MP-8_dbPP       | 15.552 | 0.21  | 15.775 | 17 | 4.581 | 0.131 | 6.113 | 25% |
| Re | MP-8_dbP        | 15.559 | 0.205 | 15.779 | 17 | 4.544 | 0.253 | 5.956 | 24% |
| Re | MP-8_db         | 15.535 | 0.208 | 15.778 | 17 | 4.554 | 0.221 | 6.195 | 26% |
| Re | MP-8_OhB        | 15.558 | 0.206 | 15.779 | 17 | 4.543 | 0.253 | 5.956 | 24% |
| Re | MP-8_Oh         | 15.769 | 0.192 | 15.67  | 17 | 6.216 | 0.352 | 6.556 | 5%  |
| Re | MP-8_TdB        | 15.556 | 0.209 | 15.775 | 17 | 4.589 | 0.115 | 6.102 | 25% |
| Re | MP-8_Td         | 15.535 | 0.208 | 15.778 | 17 | 4.554 | 0.221 | 6.195 | 26% |
| Sr | MP-76_crowdion  | 56.299 | 0.294 | 55.767 | 33 | 1.752 | 0.071 | 2.155 | 19% |
| Sr | MP-76_db100     | 56.303 | 0.274 | 55.721 | 33 | 1.762 | 0.07  | 1.952 | 10% |
| Sr | MP-76_db110     | 56.342 | 0.275 | 55.507 | 33 | 1.95  | 0.062 | 2.101 | 7%  |
| Sr | MP-76_db111     | 56.236 | 0.41  | 55.729 | 33 | 2.1   | 0.038 | 2.189 | 4%  |
| Sr | MP-76_Oh        | 56.307 | 0.274 | 55.722 | 33 | 1.762 | 0.07  | 1.952 | 10% |
| Sr | MP-76_Td        | 56.303 | 0.274 | 55.723 | 33 | 1.762 | 0.07  | 1.952 | 10% |
| Ti | MP-46_crowdionB | 16.998 | 0.087 | 17.2   | 17 | 2.265 | 0.085 | 2.489 | 9%  |
| Ti | MP-46_crowdionB | 16.979 | 0.08  | 17.076 | 17 | 3.162 | 0.127 | 2.515 | 26% |
| Ti | MP-46_crowdionP | 17.031 | 0.051 | 17.229 | 17 | 2.224 | 0.053 | 2.513 | 12% |
| Ti | MP-46_crowdion  | 17.033 | 0.052 | 17.233 | 17 | 2.221 | 0.053 | 2.517 | 12% |
| Ti | MP-46_dbB       | 16.979 | 0.08  | 17.075 | 17 | 3.162 | 0.127 | 2.515 | 26% |
| Ti | MP-46_dbP       | 16.962 | 0.034 | 17.286 | 17 | 1.702 | 0.049 | 1.225 | 39% |
| Ti | MP-46_dbPP      | 17.06  | 0.074 | 17.185 | 17 | 2.298 | 0.052 | 2.445 | 6%  |
| Ti | MP-46_dbP       | 16.962 | 0.035 | 17.289 | 17 | 1.701 | 0.049 | 1.223 | 39% |
| Ti | MP-46_db        | 16.956 | 0.069 | 17.229 | 17 | 2.327 | 0.064 | 2.47  | 6%  |
| Ti | MP-46_Ohb       | 16.964 | 0.06  | 17.151 | 33 | 2.515 | 0.271 | 2.34  | 7%  |
| Ti | MP-46_Ohp       | 16.978 | 0.069 | 17.138 | 33 | 2.729 | 0.027 | 2.217 | 23% |
| Ti | MP-46_Tdb       | 16.949 | 0.051 | 17.078 | 33 | 2.583 | 0.121 | 2.214 | 17% |
| Ti | MP-46_Tdp       | 16.966 | 0.067 | 17.077 | 33 | 2.397 | 0.147 | 2.163 | 11% |
| Zn | MP-79_crowdionB | 15.569 | 0.139 | 15.773 | 17 | 0.462 | 0.154 | 0.519 | 11% |
| Zn | MP-79_crowdionB | 15.569 | 0.139 | 15.773 | 17 | 0.462 | 0.154 | 0.519 | 11% |
| Zn | MP-79_crowdionB | 15.901 | 0.11  | 15.759 | 17 | 0.672 | 0.101 | 0.726 | 7%  |
| Zn | MP-79_crowdionB | 15.901 | 0.11  | 15.759 | 17 | 0.672 | 0.101 | 0.726 | 7%  |
| Zn | MP-79_crowdionP | 15.904 | 0.088 | 15.748 | 17 | 0.592 | 0.028 | 0.512 | 16% |
| Zn | MP-79_crowdionP | 15.904 | 0.088 | 15.748 | 17 | 0.592 | 0.028 | 0.512 | 16% |
| Zn | MP-79_crowdion  | 15.912 | 0.086 | 15.795 | 17 | 0.609 | 0.028 | 0.524 | 16% |
| Zn | MP-79_crowdion  | 15.912 | 0.086 | 15.795 | 17 | 0.609 | 0.028 | 0.524 | 16% |

|    |                  |        |       |        |    |       |       |       |     |
|----|------------------|--------|-------|--------|----|-------|-------|-------|-----|
| Zn | MP-79_dbB        | 15.654 | 0.059 | 15.565 | 17 | 0.366 | 0.042 | 0.525 | 30% |
| Zn | MP-79_dbP        | 15.911 | 0.087 | 15.794 | 17 | 0.61  | 0.029 | 0.522 | 17% |
| Zn | MP-79_dbPP       | 15.909 | 0.084 | 15.77  | 17 | 0.6   | 0.028 | 0.5   | 20% |
| Zn | MP-79_dbP        | 15.911 | 0.087 | 15.771 | 17 | 0.615 | 0.025 | 0.52  | 18% |
| Zn | MP-79_db         | 15.952 | 0.167 | 15.809 | 17 | 0.604 | 0.064 | 0.614 | 2%  |
| Zn | MP-79_OhB        | 15.911 | 0.087 | 15.769 | 17 | 0.615 | 0.026 | 0.52  | 18% |
| Zn | MP-79_Oh         | 15.796 | 0.06  | 15.675 | 17 | 0.494 | 0.043 | 0.57  | 13% |
| Zn | MP-79_TdB        | 15.911 | 0.084 | 15.773 | 17 | 0.6   | 0.027 | 0.496 | 21% |
| Zn | MP-79_Td         | 15.953 | 0.167 | 15.826 | 17 | 0.606 | 0.064 | 0.691 | 12% |
| Zr | MP-131_crowdionB | 23.634 | 0.096 | 23.595 | 17 | 0.948 | 0.095 | 0.685 | 38% |
| Zr | MP-131_crowdionB | 23.523 | 0.278 | 23.697 | 17 | 2.402 | 1.37  | 1.675 | 43% |
| Zr | MP-131_crowdion  | 23.634 | 0.097 | 23.594 | 17 | 0.949 | 0.095 | 0.687 | 38% |
| Zr | MP-131_dbB       | 23.458 | 0.078 | 23.572 | 17 | 1.813 | 0.069 | 1.561 | 16% |
| Zr | MP-131_dbP       | 23.634 | 0.094 | 23.594 | 17 | 0.948 | 0.095 | 0.688 | 38% |
| Zr | MP-131_dbPP      | 23.436 | 0.131 | 23.568 | 17 | 2.231 | 0.128 | 2.44  | 9%  |
| Zr | MP-131_dbP       | 23.635 | 0.097 | 23.596 | 17 | 0.953 | 0.095 | 0.69  | 38% |
| Zr | MP-131_db        | 23.404 | 0.114 | 23.313 | 17 | 1.397 | 0.156 | 1.685 | 17% |
| Zr | MP-131_OhB       | 23.503 | 0.135 | 23.567 | 17 | 1.61  | 0.169 | 1.796 | 10% |
| Zr | MP-131_Oh        | 23.24  | 0.073 | 23.575 | 17 | 1.406 | 0.083 | 1.747 | 20% |
| Zr | MP-131_TdB       | 23.632 | 0.097 | 23.601 | 17 | 0.948 | 0.095 | 0.687 | 38% |
| Zr | MP-131_Td        | 23.631 | 0.095 | 23.604 | 17 | 0.952 | 0.095 | 0.692 | 38% |

Interstitial atoms positions were taken from the literature references for bcc<sup>1</sup>, diamond cubic<sup>1</sup>, fcc<sup>2</sup>, and hcp<sup>3</sup>. All interstitial calculations I and Sb (bcc crystal system) were found not to be stable for both and not included in this table.

**Table S6.** DNP and DFT Elastic Constants (GPa) for ground-state lattices.

| Element | Elastic Constant | DNP  | Standard Deviation | DFT1 | MPDB-ID#  | DFT2 |
|---------|------------------|------|--------------------|------|-----------|------|
| Ag      | C11              | 128  | 17                 | 109  |           | 100  |
| Ag      | C12              | 99   | 27                 | 87   | MP-124    | 82   |
| Ag      | C44              | 42   | 2                  | 52   |           | 41   |
| Al      | C11              | 121  | 9                  | 104  |           | 107  |
| Al      | C12              | 75   | 7                  | 73   | MP-134    | 60   |
| Al      | C44              | 33   | 1                  | 32   |           | 34   |
| Au      | C11              | 150  | 12                 | 151  |           | 151  |
| Au      | C12              | 126  | 8                  | 129  | MP-81     | 129  |
| Au      | C44              | 40   | 3                  | 29   |           | 29   |
| Co      | C11              | 387  | 88                 | 358  |           | 437  |
| Co      | C12              | 273  | 74                 | 165  |           | 179  |
| Co      | C13              | 187  | 61                 | 114  | MP-54     | 143  |
| Co      | C33              | 373  | 122                | 409  |           | 485  |
| Co      | C44              | 87   | 10                 | 95   |           | 129  |
| Co      | C66              | 93   | 15                 | 96   |           | 88   |
| Cu      | C11              | 152  | 20                 | 159  |           | 153  |
| Cu      | C12              | 122  | 2                  | 129  | MP-30     | 122  |
| Cu      | C44              | 65   | 1                  | 79   |           | 87   |
| Ge      | C11              | 82   | 22                 | 104  |           | 104  |
| Ge      | C12              | 54   | 9                  | 73   | MP-32     | 37   |
| Ge      | C44              | 35   | 7                  | 32   |           | 56   |
| I       | C11              | 30   | 4                  | 55   |           | NA   |
| I       | C12              | 36   | 4                  | 40   |           | NA   |
| I       | C13              | 34   | 3                  | 0    |           | NA   |
| I       | C22              | 53   | 2                  | 55   | MP-601148 | NA   |
| I       | C33              | 64   | 4                  | 2    |           | NA   |
| I       | C44              | -28  | 9                  | 4    |           | NA   |
| I       | C55              | -7   | 2                  | 0    |           | NA   |
| I       | C66              | 6    | 2                  | 0    |           | NA   |
| Kr      | C11              | 1    | 2                  | 1    |           | -2   |
| Kr      | C12              | 1    | 1                  | 0    | MP-61211  | 0    |
| Kr      | C44              | 0    | 0                  | 0    |           | 0    |
| Li      | C11              | 13.8 | 10.5               | 15   |           | 22   |
| Li      | C12              | 12.1 | 9.8                | 13   | MP-135    | 10   |
| Li      | C44              | 12   | 0.5                | 11   |           | 18   |
| Mg      | C11              | 59   | 7                  | 58   |           |      |
| Mg      | C12              | 22   | 5                  | 30   |           |      |
| Mg      | C13              | 15   | 5                  | 22   | MP-153    |      |
| Mg      | C33              | 74   | 7                  | 66   |           |      |
| Mg      | C44              | 18   | 1                  | 20   |           |      |
| Mg      | C66              | 18   | 1                  | 14   |           |      |
| Mo      | C11              | 396  | 67                 | 472  |           |      |
| Mo      | C12              | 181  | 71                 | 158  | MP-129    |      |
| Mo      | C44              | 87   | 14                 | 106  |           |      |
| Nb      | C11              | 386  | 95                 | 472  | MP-75     | 233  |

|    |     |     |     |     |          |      |
|----|-----|-----|-----|-----|----------|------|
| Nb | C12 | 191 | 120 | 158 |          | 145  |
| Nb | C44 | 80  | 23  | 106 |          | 11   |
| Ni | C11 | 202 | 24  | 276 |          |      |
| Ni | C12 | 144 | 65  | 159 | MP-23    |      |
| Ni | C44 | 124 | 6   | 132 |          |      |
| Os | C11 | 860 | 105 | 742 |          | 730  |
| Os | C12 | 190 | 114 | 209 |          | 226  |
| Os | C13 | 270 | 125 | 240 | MP-49    | 220  |
| Os | C33 | 800 | 135 | 800 |          | 824  |
| Os | C44 | 200 | 35  | 267 |          | 252  |
| Os | C66 | 115 | 32  | 243 |          | 252  |
| Pb | C11 | 64  | 19  | 47  |          |      |
| Pb | C12 | 46  | 14  | 32  | MP-20483 |      |
| Pb | C44 | 5   | 4   | 18  |          |      |
| Pd | C11 | 222 | 42  | 209 |          | 187  |
| Pd | C12 | 149 | 56  | 150 | MP-2     | 147  |
| Pd | C44 | 75  | 10  | 63  |          | 71   |
| Pt | C11 | 310 | 17  | 303 |          | 287  |
| Pt | C12 | 150 | 19  | 220 | MP-126   | 222  |
| Pt | C44 | 73  | 5   | 54  |          | 65   |
| Re | C11 | 767 | 114 | 607 |          | 608  |
| Re | C12 | 397 | 108 | 273 |          | 283  |
| Re | C13 | 325 | 119 | 214 | MP-8     | 227  |
| Re | C33 | 784 | 88  | 670 |          | 673  |
| Re | C44 | 71  | 3   | 156 |          | 165  |
| Re | C66 | 85  | 4   | 157 |          | 161  |
| Sb | C11 | 71  | 14  | 91  |          |      |
| Sb | C12 | 35  | 6   | 24  |          |      |
| Sb | C13 | 52  | 9   | 21  |          |      |
| Sb | C22 | 71  | 14  | 91  | MP-104   |      |
| Sb | C33 | 80  | 13  | 38  |          |      |
| Sb | C44 | 13  | 7   | 27  |          |      |
| Sb | C55 | 13  | 7   | 27  |          |      |
| Sb | C66 | 18  | 5   | 34  |          |      |
| Sr | C11 | 14  | 3   | 15  |          |      |
| Sr | C12 | 11  | 2   | 10  | MP-76    |      |
| Sr | C44 | 12  | 1   | 12  |          |      |
| Ti | C11 | 257 | 84  | 177 |          |      |
| Ti | C12 | 200 | 56  | 83  |          |      |
| Ti | C13 | 140 | 74  | 76  | MP-72    |      |
| Ti | C33 | 270 | 62  | 191 |          |      |
| Ti | C44 | 24  | 2   | 42  |          |      |
| Ti | C66 | 29  | 18  | 47  |          |      |
| Zn | C11 | 122 | 9   | 163 |          | 189  |
| Zn | C12 | 82  | 4   | 45  |          | 35.9 |
| Zn | C13 | 87  | 5   | 48  | MP-79    | 36.8 |
| Zn | C33 | 104 | 16  | 61  |          | 91   |
| Zn | C44 | 12  | 2   | 32  |          | 83   |
| Zn | C66 | 20  | 4   | 59  |          | 31.3 |

|    |     |     |    |            |        |     |
|----|-----|-----|----|------------|--------|-----|
| Zr | C11 | 187 | 13 | <i>144</i> |        | 72  |
| Zr | C12 | 79  | 21 | 65         |        | 21  |
| Zr | C13 | 122 | 19 | 67         | MP-131 | 35  |
| Zr | C33 | 144 | 16 | <i>162</i> |        | 111 |
| Zr | C44 | 54  | 4  | 26         |        | 29  |
| Zr | C66 | 11  | 3  | <i>40</i>  |        | 23  |

Values in *italics* were taken from the Material Project Database in March 2023. All other values were calculated. Values in the DFT1 column were used in the comparison plot in the maintext.

**Table S7.** Additional Elastic Constants (GPA) for Trained Non-Groundstate Structures.

| Element | C <sub>xx</sub> | Structure ID                     | C <sub>xx,DNP</sub> | s.d. | C <sub>xx,DFT</sub> | Training set | C <sub>xx, DNP Error</sub> |
|---------|-----------------|----------------------------------|---------------------|------|---------------------|--------------|----------------------------|
| Ag      | C11             | MP-989737                        | 177                 | 23   |                     | Y            |                            |
| Ag      | C12             | MP-989737                        | 97                  | 26   |                     | Y            |                            |
| Ag      | C13             | MP-989737                        | 94                  | 25   |                     | Y            |                            |
| Ag      | C22             | MP-989737                        | 153                 | 16   |                     | Y            |                            |
| Ag      | C33             | MP-989737                        | 156                 | 16   |                     | Y            |                            |
| Ag      | C44             | MP-989737                        | 24                  | 5    |                     | Y            |                            |
| Ag      | C55             | MP-989737                        | 23                  | 3    |                     | Y            |                            |
| Ag      | C66             | MP-989737                        | 24                  | 3    |                     | Y            |                            |
| Ag      | C11             | MP-8566                          | 151                 | 15   | 126                 | Y            | 20%                        |
| Ag      | C12             | MP-8566                          | 102                 | 25   | 75                  | Y            | 35%                        |
| Ag      | C13             | MP-8566                          | 90                  | 25   | 59                  | Y            | 52%                        |
| Ag      | C22             | MP-8566                          | 151                 | 15   | 126                 | Y            | 20%                        |
| Ag      | C33             | MP-8566                          | 177                 | 22   | 138                 | Y            | 28%                        |
| Ag      | C44             | MP-8566                          | 23                  | 3    | 21                  | Y            | 9%                         |
| Ag      | C55             | MP-8566                          | 23                  | 3    | 21                  | Y            | 9%                         |
| Ag      | C66             | MP-8566                          | 25                  | 5    | 26                  | Y            | 5%                         |
| Ag      | C11             | MP-10597                         | 157                 | 13   | 126                 | Y            | 24%                        |
| Ag      | C12             | MP-10597                         | 108                 | 23   | 74                  | Y            | 46%                        |
| Ag      | C13             | MP-10597                         | 100                 | 26   | 60                  | Y            | 67%                        |
| Ag      | C22             | MP-10597                         | 157                 | 13   | 126                 | Y            | 24%                        |
| Ag      | C33             | MP-10597                         | 191                 | 25   | 147                 | Y            | 30%                        |
| Ag      | C44             | MP-10597                         | 23                  | 2    | 24                  | Y            | 6%                         |
| Ag      | C55             | MP-10597                         | 23                  | 2    | 24                  | Y            | 6%                         |
| Ag      | C66             | MP-10597                         | 24                  | 5    | 26                  | Y            | 7%                         |
|         |                 | ND-                              |                     |      |                     |              |                            |
| Ag      | C11             | eI8KAHKA9NeQjf48uVhI3<br>OmTw2An | 119                 | 16   | 160                 | Y            | 26%                        |
|         |                 | ND-                              |                     |      |                     |              |                            |
| Ag      | C12             | eI8KAHKA9NeQjf48uVhI3<br>OmTw2An | 55                  | 35   | 3                   | Y            | 1747%                      |
|         |                 | ND-                              |                     |      |                     |              |                            |
| Ag      | C13             | eI8KAHKA9NeQjf48uVhI3<br>OmTw2An | 45                  | 37   | 94                  | Y            | 52%                        |
|         |                 | ND-                              |                     |      |                     |              |                            |
| Ag      | C22             | eI8KAHKA9NeQjf48uVhI3<br>OmTw2An | 127                 | 51   | 180                 | Y            | 30%                        |
|         |                 | ND-                              |                     |      |                     |              |                            |
| Ag      | C33             | eI8KAHKA9NeQjf48uVhI3<br>OmTw2An | 130                 | 59   | 108                 | Y            | 21%                        |
|         |                 | ND-                              |                     |      |                     |              |                            |
| Ag      | C44             | eI8KAHKA9NeQjf48uVhI3<br>OmTw2An | 20                  | 17   | -9                  | Y            | 322%                       |
|         |                 | ND-                              |                     |      |                     |              |                            |
| Ag      | C55             | eI8KAHKA9NeQjf48uVhI3<br>OmTw2An | 15                  | 17   | -24                 | Y            | 164%                       |
|         |                 | ND-                              |                     |      |                     |              |                            |
| Ag      | C66             | eI8KAHKA9NeQjf48uVhI3<br>OmTw2An | -26                 | 107  | 43                  | Y            | 161%                       |
| Al      | C11             | sc                               | 66                  | 44   | 110                 | Y            | 40%                        |

|    |     |                                 |     |     |     |   |      |
|----|-----|---------------------------------|-----|-----|-----|---|------|
| Al | C12 | sc                              | 58  | 28  | 32  | Y | 81%  |
| Al | C44 | sc                              | 12  | 4   | -13 | Y | 188% |
| Al | C11 | MP-1183144                      | 136 | 10  | 121 | Y | 12%  |
| Al | C12 | MP-1183144                      | 73  | 8   | 57  | Y | 27%  |
| Al | C13 | MP-1183144                      | 65  | 10  | 56  | Y | 17%  |
| Al | C22 | MP-1183144                      | 136 | 10  | 124 | Y | 9%   |
| Al | C33 | MP-1183144                      | 130 | 13  | 108 | Y | 20%  |
| Al | C44 | MP-1183144                      | 24  | 1   | 35  | Y | 33%  |
| Al | C55 | MP-1183144                      | 24  | 1   | 30  | Y | 21%  |
| Al | C66 | MP-1183144                      | 32  | 1   | 30  | Y | 5%   |
| Al | C11 | MP-998860                       | 72  | 23  | 40  | Y | 80%  |
| Al | C12 | MP-998860                       | 68  | 14  | 90  | Y | 24%  |
| Al | C44 | MP-998860                       | 40  | 1   | 34  | Y | 17%  |
| Al | C11 | MP-1239196                      | 77  | 18  | 58  | Y | 33%  |
| Al | C12 | MP-1239196                      | 60  | 13  | 42  | Y | 42%  |
| Al | C13 | MP-1239196                      | 48  | 17  | 26  | Y | 86%  |
| Al | C22 | MP-1239196                      | 77  | 18  | 58  | Y | 33%  |
| Al | C33 | MP-1239196                      | 76  | 21  | 152 | Y | 50%  |
| Al | C44 | MP-1239196                      | 7   | 1   | 32  | Y | 79%  |
| Al | C55 | MP-1239196                      | 7   | 1   | 21  | Y | 69%  |
| Al | C66 | MP-1239196                      | 12  | 1   | 21  | Y | 43%  |
| Au | C11 | MP-1008634                      | 244 | 112 | 178 | Y | 37%  |
| Au | C12 | MP-1008634                      | 163 | 107 | 131 | Y | 25%  |
| Au | C13 | MP-1008634                      | 188 | 107 | 107 | Y | 75%  |
| Au | C22 | MP-1008634                      | 244 | 112 | 178 | Y | 37%  |
| Au | C33 | MP-1008634                      | 220 | 112 | 174 | Y | 26%  |
| Au | C44 | MP-1008634                      | 40  | 3   | 19  | Y | 112% |
| Au | C55 | MP-1008634                      | 40  | 3   | 19  | Y | 112% |
| Au | C66 | MP-1008634                      | 16  | 4   | 24  | Y | 33%  |
| Au | C11 | ND-Vm5tz1VwY8ikjDNa-7trkwSIVnb6 | 116 | 29  | 149 | Y | 22%  |
| Au | C12 | ND-Vm5tz1VwY8ikjDNa-7trkwSIVnb7 | 104 | 45  | 135 | Y | 23%  |
| Au | C44 | ND-Vm5tz1VwY8ikjDNa-7trkwSIVnb8 | 13  | 1   | 51  | Y | 75%  |
| Au | C11 | ND-j9Rw6C2osMGGmW84YS-gThlwm-YL | 258 | 132 | 135 | Y | 91%  |
| Au | C12 | ND-j9Rw6C2osMGGmW84YS-gThlwm-YL | 201 | 128 | 137 | Y | 47%  |
| Au | C13 | ND-j9Rw6C2osMGGmW84YS-gThlwm-YL | 189 | 126 | 134 | Y | 41%  |
| Au | C22 | ND-j9Rw6C2osMGGmW84YS-gThlwm-YL | 258 | 132 | 135 | Y | 91%  |
| Au | C33 | ND-j9Rw6C2osMGGmW84YS-gThlwm-YL | 276 | 126 | 177 | Y | 56%  |
| Au | C44 | ND-j9Rw6C2osMGGmW84YS-gThlwm-YL | 27  | 3   | 54  | Y | 49%  |



|    |     |   |       |           |     |   |        |
|----|-----|---|-------|-----------|-----|---|--------|
| Au | C55 | ND-<br>j9Rw6C2osMGGmW84YS-<br>gThlwm-YL | 27    | 3         | 14  | Y | 96%    |
| Au | C66 | ND-<br>j9Rw6C2osMGGmW84YS-<br>gThlwm-YL | 29    | 2         | 14  | Y | 104%   |
| Au | C11 | sc                                      | 247   | 108       | 201 | Y | 23%    |
| Au | C12 | sc                                      | 172   | 102       | 128 | Y | 34%    |
| Au | C44 | sc                                      | 27    | 3         | 22  | Y | 20%    |
| Co | C11 | MP-102                                  | 390   | 83        | 325 | Y | 20%    |
| Co | C12 | MP-102                                  | 495   | 176       | 137 | Y | 262%   |
| Co | C44 | MP-102                                  | 108   | 27        | 162 | Y | 33%    |
| Co | C11 | MP-1271679                              | 89990 | 763<br>35 | 362 | Y | 24759% |
| Co | C12 | MP-1271679                              | 88973 | 755<br>20 | 134 | Y | 66297% |
| Co | C13 | MP-1271679                              | 89780 | 761<br>98 | 107 | Y | 83806% |
| Co | C22 | MP-1271679                              | 88606 | 748<br>14 | 361 | Y | 24445% |
| Co | C33 | MP-1271679                              | 89990 | 763<br>34 | 354 | Y | 25321% |
| Co | C44 | MP-1271679                              | 164   | 81        | 114 | Y | 44%    |
| Co | C55 | MP-1271679                              | 109   | 72        | 62  | Y | 75%    |
| Co | C66 | MP-1271679                              | 166   | 83        | 64  | Y | 159%   |
| Co | C11 | MP-1193227                              | 224   | 100       | 244 | Y | 8%     |
| Co | C12 | MP-1193227                              | 145   | 89        | 209 | Y | 31%    |
| Co | C13 | MP-1193227                              | 84    | 95        | 109 | Y | 23%    |
| Co | C22 | MP-1193227                              | 224   | 100       | 243 | Y | 8%     |
| Co | C33 | MP-1193227                              | 319   | 115       | 316 | Y | 1%     |
| Co | C44 | MP-1193227                              | 26    | 13        | 40  | Y | 36%    |
| Co | C55 | MP-1193227                              | 26    | 13        | 1   | Y | 2450%  |
| Co | C66 | MP-1193227                              | 41    | 10        | 3   | Y | 1260%  |
| Co | C11 | sc                                      | 186   | 39        | -27 | Y | 787%   |
| Co | C12 | sc                                      | 88    | 18        | 12  | Y | 629%   |
| Co | C44 | sc                                      | 15    | 6         | 7   | Y | 111%   |
| Cu | C11 | MP-989695                               | 239   | 20        | 219 | Y | 9%     |
| Cu | C12 | MP-989695                               | 148   | 19        | 122 | Y | 21%    |
| Cu | C13 | MP-989695                               | 116   | 21        | 90  | Y | 29%    |
| Cu | C22 | MP-989695                               | 239   | 20        | 216 | Y | 11%    |
| Cu | C33 | MP-989695                               | 273   | 17        | 244 | Y | 12%    |
| Cu | C44 | MP-989695                               | 44    | 2         | 45  | Y | 3%     |
| Cu | C55 | MP-989695                               | 44    | 2         | 33  | Y | 32%    |
| Cu | C66 | MP-989695                               | 46    | 1         | 33  | Y | 38%    |
| Cu | C11 | MP-1010136                              | 258   | 29        | 145 | Y | 78%    |
| Cu | C12 | MP-1010136                              | 107   | 30        | 140 | Y | 24%    |
| Cu | C13 | MP-1010136                              | 114   | 28        | 146 | Y | 22%    |
| Cu | C22 | MP-1010136                              | 216   | 34        | 145 | Y | 49%    |
| Cu | C33 | MP-1010136                              | 239   | 25        | 161 | Y | 49%    |
| Cu | C44 | MP-1010136                              | 58    | 5         | 77  | Y | 25%    |
| Cu | C55 | MP-1010136                              | 37    | 1         | 50  | Y | 27%    |
| Cu | C66 | MP-1010136                              | 32    | 13        | 51  | Y | 37%    |

|    |     |            |     |     |     |   |       |
|----|-----|------------|-----|-----|-----|---|-------|
| Cu | C11 | MP-998890  | 196 | 143 | 214 | Y | 9%    |
| Cu | C12 | MP-998890  | 161 | 71  | 121 | Y | 33%   |
| Cu | C44 | MP-998890  | 41  | 9   | 90  | Y | 54%   |
| Cu | C11 | MP-1120774 | 106 | 5   |     | Y |       |
| Cu | C12 | MP-1120774 | 49  | 3   |     | Y |       |
| Cu | C13 | MP-1120774 | 0   | 0   |     | Y |       |
| Cu | C22 | MP-1120774 | 106 | 5   |     | Y |       |
| Cu | C33 | MP-1120774 | 0   | 0   |     | Y |       |
| Cu | C44 | MP-1120774 | 0   | 0   |     | Y |       |
| Cu | C55 | MP-1120774 | 0   | 0   |     | Y |       |
| Cu | C66 | MP-1120774 | 29  | 1   |     | Y |       |
| Ge | C11 | MP-1224349 | 166 | 65  | 116 | N | 43%   |
| Ge | C12 | MP-1224349 | 117 | 49  | 74  | N | 58%   |
| Ge | C13 | MP-1224349 | 81  | 58  | 7   | N | 1063% |
| Ge | C22 | MP-1224349 | 163 | 63  | 69  | N | 136%  |
| Ge | C33 | MP-1224349 | 189 | 113 | 169 | N | 12%   |
| Ge | C44 | MP-1224349 | 29  | 14  | -20 | N | 246%  |
| Ge | C55 | MP-1224349 | 29  | 15  | 20  | N | 45%   |
| Ge | C66 | MP-1224349 | 22  | 8   | 19  | N | 16%   |
| Ge | C11 | MP-1091415 | 95  | 13  | 130 | Y | 27%   |
| Ge | C12 | MP-1091415 | 59  | 11  | 33  | Y | 79%   |
| Ge | C13 | MP-1091415 | 39  | 19  | 20  | Y | 95%   |
| Ge | C22 | MP-1091415 | 95  | 13  | 130 | Y | 27%   |
| Ge | C33 | MP-1091415 | 159 | 13  | 143 | Y | 11%   |
| Ge | C44 | MP-1091415 | 17  | 1   | 48  | Y | 65%   |
| Ge | C55 | MP-1091415 | 17  | 1   | 40  | Y | 58%   |
| Ge | C66 | MP-1091415 | 18  | 1   | 40  | Y | 55%   |
| Ge | C11 | MP-1007760 | 109 | 14  | 127 | N | 14%   |
| Ge | C12 | MP-1007760 | 67  | 14  | 32  | N | 108%  |
| Ge | C13 | MP-1007760 | 45  | 23  | 17  | N | 167%  |
| Ge | C44 | MP-1007760 | 22  | 3   | 37  | N | 41%   |
| Ge | C11 | MP-1198022 | 100 | 33  | 104 | N | 4%    |
| Ge | C12 | MP-1198022 | 50  | 26  | 73  | N | 32%   |
| Ge | C13 | MP-1198022 | 50  | 25  | 73  | N | 32%   |
| Ge | C22 | MP-1198022 | 100 | 33  | 104 | N | 4%    |
| Ge | C33 | MP-1198022 | 100 | 33  | 104 | N | 4%    |
| Ge | C44 | MP-1198022 | 25  | 3   | 32  | N | 22%   |
| Ge | C55 | MP-1198022 | 25  | 3   | 32  | N | 22%   |
| Ge | C66 | MP-1198022 | 25  | 3   | 32  | N | 22%   |
| Ge | C11 | MP-128     | 69  | 16  | 114 | N | 40%   |
| Ge | C12 | MP-128     | 14  | 17  | 26  | N | 48%   |
| Ge | C13 | MP-128     | 20  | 17  | 29  | N | 31%   |
| Ge | C22 | MP-128     | 76  | 18  | 114 | N | 34%   |
| Ge | C33 | MP-128     | 77  | 24  | 75  | N | 2%    |
| Ge | C44 | MP-128     | 22  | 4   | 40  | N | 45%   |
| Ge | C55 | MP-128     | 27  | 5   | 40  | N | 33%   |
| Ge | C66 | MP-128     | 21  | 2   | 44  | N | 53%   |
| Ge | C11 | MP-137     | 92  | 24  | 140 | Y | 34%   |
| Ge | C12 | MP-137     | 36  | 5   | 15  | Y | 139%  |
| Ge | C44 | MP-137     | 28  | 6   | 44  | Y | 36%   |

|    |     |            |     |     |      |   |         |
|----|-----|------------|-----|-----|------|---|---------|
| Ge | C11 | MP-78      | 112 | 6   | 99   | Y | 13%     |
| Ge | C12 | MP-78      | 39  | 6   | 48   | Y | 20%     |
| Ge | C13 | MP-78      | 53  | 8   | 48   | Y | 11%     |
| Ge | C22 | MP-78      | 80  | 18  | 98   | Y | 19%     |
| Ge | C33 | MP-78      | 121 | 11  | 98   | Y | 23%     |
| Ge | C44 | MP-78      | 25  | 7   | 47   | Y | 48%     |
| Ge | C55 | MP-78      | 26  | 24  | 36   | Y | 27%     |
| Ge | C66 | MP-78      | 27  | 1   | 36   | Y | 24%     |
| Ge | C11 | MP-1061054 | 111 | 7   | -537 | N | 121%    |
| Ge | C12 | MP-1061054 | 50  | 6   | 267  | N | 81%     |
| Ge | C13 | MP-1061054 | 41  | 4   | 98   | N | 59%     |
| Ge | C22 | MP-1061054 | 108 | 2   | 3    | N | 3493%   |
| Ge | C33 | MP-1061054 | 85  | 13  | 34   | N | 150%    |
| Ge | C44 | MP-1061054 | 26  | 3   | -74  | N | 134%    |
| Ge | C55 | MP-1061054 | 28  | 1   | -337 | N | 108%    |
| Ge | C66 | MP-1061054 | 31  | 16  | -77  | N | 140%    |
| Ge | C11 | MP-148     | 133 | 86  |      | N |         |
| Ge | C12 | MP-148     | 64  | 52  |      | N |         |
| Ge | C13 | MP-148     | 64  | 53  |      | N |         |
| Ge | C22 | MP-148     | 136 | 75  |      | N |         |
| Ge | C33 | MP-148     | 133 | 73  |      | N |         |
| Ge | C44 | MP-148     | 34  | 25  |      | N |         |
| Ge | C55 | MP-148     | 27  | 4   |      | N |         |
| Ge | C66 | MP-148     | 28  | 4   |      | N |         |
| Ge | C11 | bcc        | 106 | 32  | 514  | N | 79%     |
| Ge | C12 | bcc        | 100 | 33  | 477  | N | 79%     |
| Ge | C44 | bcc        | 19  | 8   | 273  | N | 93%     |
| Ge | C11 | sc         | 178 | 49  | 30   | N | 493%    |
| Ge | C12 | sc         | 57  | 6   | 34   | N | 67%     |
| Ge | C44 | sc         | 10  | 3   | 19   | N | 49%     |
| I  | C11 | MP-23153   | 32  | 14  | 2    | Y | 1495%   |
| I  | C12 | MP-23153   | 24  | 14  | -1   | Y | 2470%   |
| I  | C13 | MP-23153   | 21  | 14  | 0    | Y |         |
| I  | C22 | MP-23153   | 32  | 14  | 29   | Y | 9%      |
| I  | C33 | MP-23153   | 90  | 88  | 15   | Y | 501%    |
| I  | C44 | MP-23153   | 60  | 71  | 19   | Y | 215%    |
| I  | C55 | MP-23153   | 2   | 7   | 1    | Y | 80%     |
| I  | C66 | MP-23153   | 4   | 1   | 0    | Y | #DIV/0! |
| I  | C11 | MP-1180981 | 44  | 21  | 42   | Y | 5%      |
| I  | C12 | MP-1180981 | 36  | 10  | 49   | Y | 27%     |
| I  | C13 | MP-1180981 | 37  | 28  | 0    | Y |         |
| I  | C22 | MP-1180981 | 96  | 79  | 46   | Y | 109%    |
| I  | C33 | MP-1180981 | 152 | 113 | 1    | Y | 15050%  |
| I  | C44 | MP-1180981 | 2   | 0   | -64  | Y | 103%    |
| I  | C55 | MP-1180981 | 18  | 16  | 0    | Y |         |
| I  | C66 | MP-1180981 | 8   | 12  | 0    | Y |         |
| I  | C11 | MP-601148  | 30  | 4   | 55   | Y | 45%     |
| I  | C12 | MP-601148  | 36  | 4   | 40   | Y | 11%     |
| I  | C13 | MP-601148  | 34  | 3   | 0    | Y |         |
| I  | C22 | MP-601148  | 53  | 2   | 55   | Y | 4%      |

|    |     |            |     |    |     |   |       |
|----|-----|------------|-----|----|-----|---|-------|
| I  | C33 | MP-601148  | 64  | 4  | 2   | Y | 3080% |
| I  | C44 | MP-601148  | -28 | 9  | 4   | Y | 793%  |
| I  | C55 | MP-601148  | -7  | 2  | 0   | Y |       |
| I  | C66 | MP-601148  | 6   | 2  | 0   | Y |       |
| I  | C11 | MP-684663  | 228 | 86 | 27  | Y | 743%  |
| I  | C12 | MP-684663  | 203 | 94 | 26  | Y | 682%  |
| I  | C44 | MP-684663  | 2   | 12 | -53 | Y | 104%  |
| Kr | C11 | MP-975590  | 9   | 15 | 1   | Y | 750%  |
| Kr | C12 | MP-975590  | 4   | 8  | 0   | Y |       |
| Kr | C13 | MP-975590  | 5   | 8  | 0   | Y |       |
| Kr | C22 | MP-975590  | 10  | 16 | 1   | Y | 850%  |
| Kr | C33 | MP-975590  | 10  | 17 | 3   | Y | 227%  |
| Kr | C44 | MP-975590  | 2   | 3  | 0   | Y |       |
| Kr | C55 | MP-975590  | 1   | 2  | 1   | Y | 20%   |
| Kr | C66 | MP-975590  | 1   | 1  | 0   | Y |       |
| Kr | C11 | MP-976347  | 11  | 18 |     | Y |       |
| Kr | C12 | MP-976347  | 5   | 9  |     | Y |       |
| Kr | C13 | MP-976347  | 4   | 6  |     | Y |       |
| Kr | C22 | MP-976347  | 9   | 16 |     | Y |       |
| Kr | C33 | MP-976347  | 5   | 9  |     | Y |       |
| Kr | C44 | MP-976347  | 1   | 1  |     | Y |       |
| Kr | C55 | MP-976347  | 1   | 1  |     | Y |       |
| Kr | C66 | MP-976347  | 2   | 3  |     | Y |       |
| Kr | C11 | MP-567365  | 12  | 20 | 4   | Y | 195%  |
| Kr | C12 | MP-567365  | 5   | 8  | 0   | Y |       |
| Kr | C13 | MP-567365  | 3   | 6  | 0   | Y |       |
| Kr | C22 | MP-567365  | 9   | 15 | 1   | Y | 770%  |
| Kr | C33 | MP-567365  | 5   | 8  | -1  | Y | 560%  |
| Kr | C44 | MP-567365  | 1   | 1  | 0   | Y |       |
| Kr | C55 | MP-567365  | 1   | 1  | 0   | Y |       |
| Kr | C66 | MP-567365  | 1   | 3  | 0   | Y |       |
| Li | C11 | MP-1018134 | 32  | 1  | 21  | Y | 50%   |
| Li | C12 | MP-1018134 | 7   | 3  | 9   | Y | 20%   |
| Li | C13 | MP-1018134 | 6   | 3  | 7   | Y | 16%   |
| Li | C22 | MP-1018134 | 21  | 3  | 21  | Y | 0%    |
| Li | C33 | MP-1018134 | 22  | 3  | 20  | Y | 10%   |
| Li | C44 | MP-1018134 | 2   | 1  | 6   | Y | 63%   |
| Li | C55 | MP-1018134 | 4   | 0  | 6   | Y | 28%   |
| Li | C66 | MP-1018134 | 5   | 0  | 6   | Y | 17%   |
| Li | C11 | MP-976411  | 21  | 5  | 23  |   | 9%    |
| Li | C12 | MP-976411  | 17  | 3  | 11  |   | 55%   |
| Li | C13 | MP-976411  | 5   | 4  | 8   |   | 34%   |
| Li | C22 | MP-976411  | 21  | 5  | 23  |   | 9%    |
| Li | C33 | MP-976411  | 33  | 3  | 23  |   | 45%   |
| Li | C44 | MP-976411  | 4   | 0  | -1  |   | 540%  |
| Li | C55 | MP-976411  | 4   | 0  | -1  |   | 540%  |
| Li | C66 | MP-976411  | 2   | 1  | 6   |   | 68%   |
| Li | C11 | MP-51      | 50  | 30 | 16  |   | 214%  |
| Li | C12 | MP-51      | 31  | 29 | 13  |   | 138%  |
| Li | C44 | MP-51      | 5   | 0  | 9   |   | 40%   |

|    |     |            |      |          |     |   |       |
|----|-----|------------|------|----------|-----|---|-------|
| Li | C11 | MP-1063005 | 25   | 10       | 28  | Y | 11%   |
| Li | C12 | MP-1063005 | 8    | 10       | 13  | Y | 35%   |
| Li | C13 | MP-1063005 | 5    | 10       | 1   | Y | 360%  |
| Li | C22 | MP-1063005 | 25   | 10       | 27  | Y | 8%    |
| Li | C33 | MP-1063005 | 29   | 10       | 37  | Y | 23%   |
| Li | C44 | MP-1063005 | 5    | 0        | 3   | Y | 53%   |
| Li | C55 | MP-1063005 | 5    | 0        | 3   | Y | 53%   |
| Li | C66 | MP-1063005 | 8    | 0        | 3   | Y | 177%  |
| Mg | C11 | MP-1056702 | 60   | 3        |     | Y |       |
| Mg | C12 | MP-1056702 | 16   | 3        |     | Y |       |
| Mg | C13 | MP-1056702 | 11   | 3        |     | Y |       |
| Mg | C22 | MP-1056702 | 60   | 3        |     | Y |       |
| Mg | C33 | MP-1056702 | 65   | 3        |     | Y |       |
| Mg | C44 | MP-1056702 | 17   | 1        |     | Y |       |
| Mg | C55 | MP-1056702 | 17   | 1        |     | Y |       |
| Mg | C66 | MP-1056702 | 19   | 1        |     | Y |       |
| Mg | C11 | MP-1094122 | 69   | 5        |     | Y |       |
| Mg | C12 | MP-1094122 | 15   | 4        |     | Y |       |
| Mg | C13 | MP-1094122 | 14   | 4        |     | Y |       |
| Mg | C22 | MP-1094122 | 58   | 5        |     | Y |       |
| Mg | C33 | MP-1094122 | 60   | 5        |     | Y |       |
| Mg | C44 | MP-1094122 | 19   | 1        |     | Y |       |
| Mg | C55 | MP-1094122 | 17   | 1        |     | Y |       |
| Mg | C66 | MP-1094122 | 18   | 1        |     | Y |       |
| Mg | C11 | MP-973364  | 60   | 3        | 61  | Y | 2%    |
| Mg | C12 | MP-973364  | 6    | 3        | 26  | Y | 78%   |
| Mg | C13 | MP-973364  | 21   | 2        | 20  | Y | 4%    |
| Mg | C22 | MP-973364  | 60   | 3        | 61  | Y | 2%    |
| Mg | C33 | MP-973364  | 45   | 4        | 66  | Y | 32%   |
| Mg | C44 | MP-973364  | 27   | 1        | 16  | Y | 68%   |
| Mg | C55 | MP-973364  | 27   | 1        | 16  | Y | 68%   |
| Mg | C66 | MP-973364  | 12   | 1        | 17  | Y | 29%   |
| Mg | C11 | MP-1247180 | 60   | 6        |     | Y |       |
| Mg | C12 | MP-1247180 | 15   | 5        |     | Y |       |
| Mg | C13 | MP-1247180 | 22   | 4        |     | Y |       |
| Mg | C22 | MP-1247180 | 74   | 7        |     | Y |       |
| Mg | C33 | MP-1247180 | 59   | 7        |     | Y |       |
| Mg | C44 | MP-1247180 | 18   | 1        |     | Y |       |
| Mg | C55 | MP-1247180 | 18   | 1        |     | Y |       |
| Mg | C66 | MP-1247180 | 18   | 1        |     | Y |       |
| Mo | C11 | sc         | 324  | 219      | 333 | Y | 3%    |
| Mo | C12 | sc         | 194  | 228      | 116 | Y | 68%   |
| Mo | C44 | sc         | -21  | 38       | -56 | Y | 63%   |
| Mo | C11 | MP-8637    | 1558 | 163<br>4 | 105 | Y | 1383% |
| Mo | C12 | MP-8637    | 1384 | 161<br>2 | 312 | Y | 344%  |
| Mo | C44 | MP-8637    | 87   | 15       | -7  | Y | 1340% |
| Mo | C11 | MP-1056004 | 372  | 167      | 215 | Y | 73%   |
| Mo | C12 | MP-1056004 | 211  | 157      | 321 | Y | 34%   |
| Mo | C13 | MP-1056004 | 246  | 149      | 112 | Y | 119%  |

|    |     |            |      |          |      |   |        |
|----|-----|------------|------|----------|------|---|--------|
| Mo | C22 | MP-1056004 | 359  | 173      | 220  | Y | 63%    |
| Mo | C33 | MP-1056004 | 523  | 129      | 430  | Y | 22%    |
| Mo | C44 | MP-1056004 | 37   | 17       | -46  | Y | 180%   |
| Mo | C55 | MP-1056004 | 38   | 10       | -72  | Y | 153%   |
| Mo | C66 | MP-1056004 | 76   | 12       | -72  | Y | 205%   |
| Nb | C11 | MP-8636    | 386  | 95       | -32  | Y | 1305%  |
| Nb | C12 | MP-8636    | 191  | 119      | 266  | Y | 28%    |
| Nb | C44 | MP-8636    | 97   | 31       | -32  | Y | 404%   |
| Nb | C11 | sc         | 1791 | 267<br>1 | 130  | Y | 1277%  |
| Nb | C12 | sc         | 606  | 867      | 131  | Y | 363%   |
| Nb | C44 | sc         | 28   | 15       | -136 | Y | 120%   |
| Ni | C11 | MP-10257   | 251  | 32       | 320  | Y | 22%    |
| Ni | C12 | MP-10257   | 85   | 31       | 142  | Y | 40%    |
| Ni | C13 | MP-10257   | 34   | 30       | 128  | Y | 74%    |
| Ni | C22 | MP-10257   | 251  | 32       | 320  | Y | 22%    |
| Ni | C33 | MP-10257   | 253  | 22       | 336  | Y | 25%    |
| Ni | C44 | MP-10257   | 71   | 6        | 55   | Y | 29%    |
| Ni | C55 | MP-10257   | 71   | 6        | 55   | Y | 29%    |
| Ni | C66 | MP-10257   | 83   | 2        | 89   | Y | 7%     |
| Ni | C11 | MP-1008728 | 137  | 80       | 143  | Y | 4%     |
| Ni | C12 | MP-1008728 | 100  | 23       | 213  | Y | 53%    |
| Ni | C44 | MP-1008728 | 97   | 39       | 152  | Y | 36%    |
| Ni | C11 | MP-1014111 | 251  | 32       | 117  | Y | 114%   |
| Ni | C12 | MP-1014111 | 85   | 31       | 35   | Y | 144%   |
| Ni | C13 | MP-1014111 | 34   | 30       | 0    | Y |        |
| Ni | C22 | MP-1014111 | 251  | 32       | 117  | Y | 114%   |
| Ni | C33 | MP-1014111 | 253  | 22       | 1    | Y | 25200% |
| Ni | C44 | MP-1014111 | 71   | 6        | 0    | Y |        |
| Ni | C55 | MP-1014111 | 71   | 6        | 0    | Y |        |
| Ni | C66 | MP-1014111 | 83   | 2        | 41   | Y | 101%   |
| Ni | C11 | MP-1094136 | 275  | 28       | 335  | Y | 18%    |
| Ni | C12 | MP-1094136 | 75   | 22       | 139  | Y | 46%    |
| Ni | C13 | MP-1094136 | 51   | 20       | 137  | Y | 63%    |
| Ni | C22 | MP-1094136 | 275  | 28       | 351  | Y | 22%    |
| Ni | C33 | MP-1094136 | 299  | 30       | 350  | Y | 15%    |
| Ni | C44 | MP-1094136 | 76   | 3        | 79   | Y | 4%     |
| Ni | C55 | MP-1094136 | 76   | 3        | 60   | Y | 26%    |
| Ni | C66 | MP-1094136 | 106  | 5        | 78   | Y | 36%    |
| Os | C11 | MP-8643    | 2764 | 142<br>6 | 569  | Y | 386%   |
| Os | C12 | MP-8643    | 2527 | 146<br>1 | 315  | Y | 702%   |
| Os | C13 | MP-8643    | 2509 | 146<br>4 | 315  | Y | 696%   |
| Os | C22 | MP-8643    | 2764 | 142<br>6 | 569  | Y | 386%   |
| Os | C33 | MP-8643    | 2782 | 142<br>4 | 561  | Y | 396%   |
| Os | C44 | MP-8643    | 100  | 21       | 285  | Y | 65%    |
| Os | C55 | MP-8643    | 100  | 21       | 283  | Y | 65%    |
| Os | C66 | MP-8643    | 110  | 28       | 283  | Y | 61%    |

|    |     |               |      |     |     |   |       |
|----|-----|---------------|------|-----|-----|---|-------|
| Os | C11 | MP-1080694    | 1588 | 782 |     | Y |       |
| Os | C12 | MP-1080694    | 1404 | 769 |     | Y |       |
| Os | C13 | MP-1080694    | 1400 | 769 |     | Y |       |
| Os | C22 | MP-1080694    | 1604 | 778 |     | Y |       |
| Os | C33 | MP-1080694    | 1516 | 763 |     | Y |       |
| Os | C44 | MP-1080694    | 67   | 21  |     | Y |       |
| Os | C55 | MP-1080694    | 39   | 18  |     | Y |       |
| Os | C66 | MP-1080694    | 75   | 11  |     | Y |       |
| Os | C11 | ND-w3arEIPCdT | 1933 | 211 |     | Y |       |
|    |     |               |      | 2   |     |   |       |
| Os | C12 | ND-w3arEIPCdT | 1835 | 217 |     | Y |       |
|    |     |               |      | 5   |     |   |       |
| Os | C13 | ND-w3arEIPCdT | 1814 | 217 |     | Y |       |
|    |     |               |      | 2   |     |   |       |
| Os | C22 | ND-w3arEIPCdT | 1930 | 214 |     | Y |       |
|    |     |               |      | 3   |     |   |       |
| Os | C33 | ND-w3arEIPCdT | 1995 | 215 |     | Y |       |
|    |     |               |      | 2   |     |   |       |
| Os | C44 | ND-w3arEIPCdT | 111  | 22  |     | Y |       |
| Os | C55 | ND-w3arEIPCdT | 40   | 20  |     | Y |       |
| Os | C66 | ND-w3arEIPCdT | 63   | 14  |     | Y |       |
| Os | C11 | ND-5FQY1      | 2764 | 142 | 731 | Y | 278%  |
|    |     |               |      | 6   |     |   |       |
| Os | C12 | ND-5FQY2      | 2527 | 146 | 260 | Y | 872%  |
|    |     |               |      | 1   |     |   |       |
| Os | C13 | ND-5FQY3      | 2509 | 146 | 202 | Y | 1142% |
|    |     |               |      | 4   |     |   |       |
| Os | C22 | ND-5FQY4      | 2764 | 142 | 737 | Y | 275%  |
|    |     |               |      | 6   |     |   |       |
| Os | C33 | ND-5FQY5      | 2782 | 142 | 801 | Y | 247%  |
|    |     |               |      | 4   |     |   |       |
| Os | C44 | ND-5FQY6      | 100  | 21  | 236 | Y | 57%   |
| Os | C55 | ND-5FQY7      | 100  | 21  | 204 | Y | 51%   |
| Os | C66 | ND-5FQY8      | 119  | 35  | 204 | Y | 42%   |
| Pb | C11 | MP-1186444    | 62   | 20  | 29  | Y | 115%  |
| Pb | C12 | MP-1186444    | 50   | 14  | 51  | Y | 2%    |
| Pb | C13 | MP-1186444    | 46   | 14  | 45  | Y | 1%    |
| Pb | C22 | MP-1186444    | 62   | 20  | 32  | Y | 95%   |
| Pb | C33 | MP-1186444    | 66   | 9   | 5   | Y | 1212% |
| Pb | C44 | MP-1186444    | 8    | 2   | -11 | Y | 173%  |
| Pb | C55 | MP-1186444    | 8    | 2   | -3  | Y | 367%  |
| Pb | C66 | MP-1186444    | 6    | 4   | -3  | Y | 307%  |
| Pb | C11 | MP-22692      | 30   | 11  | 16  | Y | 89%   |
| Pb | C12 | MP-22692      | 11   | 3   | 49  | Y | 78%   |
| Pb | C44 | MP-22692      | 6    | 2   | 18  | Y | 68%   |
| Pb | C11 | MP-1057273    | 225  | 280 | 104 | Y | 116%  |
| Pb | C12 | MP-1057273    | 111  | 137 | 73  | Y | 53%   |
| Pb | C13 | MP-1057273    | -58  | 127 | 73  | Y | 179%  |
| Pb | C22 | MP-1057273    | 63   | 6   | 104 | Y | 39%   |
| Pb | C33 | MP-1057273    | 37   | 16  | 104 | Y | 65%   |
| Pb | C44 | MP-1057273    | 55   | 90  | 32  | Y | 73%   |
| Pb | C55 | MP-1057273    | 4    | 2   | 32  | Y | 89%   |

|    |     |                |     |     |     |   |       |
|----|-----|----------------|-----|-----|-----|---|-------|
| Pb | C66 | MP-1057273     | 13  | 2   | 32  | Y | 60%   |
| Pb | C11 | MP-1247117     | 131 | 100 | 36  | Y | 265%  |
| Pb | C12 | MP-1247117     | 42  | 26  | 19  | Y | 123%  |
| Pb | C13 | MP-1247117     | 86  | 51  | 22  | Y | 289%  |
| Pb | C22 | MP-1247117     | 24  | 88  | 38  | Y | 37%   |
| Pb | C33 | MP-1247117     | 76  | 9   | 35  | Y | 117%  |
| Pb | C44 | MP-1247117     | 8   | 3   | 5   | Y | 62%   |
| Pb | C55 | MP-1247117     | 6   | 6   | 5   | Y | 12%   |
| Pb | C66 | MP-1247117     | 11  | 4   | 7   | Y | 61%   |
| Pd | C11 | MP-1186427     | 272 | 30  | 221 | Y | 23%   |
| Pd | C12 | MP-1186427     | 165 | 45  | 167 | Y | 1%    |
| Pd | C13 | MP-1186427     | 133 | 46  | 119 | Y | 12%   |
| Pd | C22 | MP-1186427     | 272 | 30  | 205 | Y | 32%   |
| Pd | C33 | MP-1186427     | 226 | 49  | 250 | Y | 10%   |
| Pd | C44 | MP-1186427     | 39  | 5   | 27  | Y | 46%   |
| Pd | C55 | MP-1186427     | 39  | 5   | 33  | Y | 19%   |
| Pd | C66 | MP-1186427     | 53  | 8   | 33  | Y | 61%   |
| Pd | C11 | ND-AzTtp       | 263 | 45  | 249 | Y | 6%    |
| Pd | C12 | ND-AzTtp       | 117 | 55  | 127 | Y | 8%    |
| Pd | C13 | ND-AzTtp       | 142 | 55  | 135 | Y | 5%    |
| Pd | C22 | ND-AzTtp       | 271 | 45  | 252 | Y | 7%    |
| Pd | C33 | ND-AzTtp       | 246 | 43  | 243 | Y | 1%    |
| Pd | C44 | ND-AzTtp       | 58  | 8   | 32  | Y | 81%   |
| Pd | C55 | ND-AzTtp       | 68  | 9   | 45  | Y | 50%   |
| Pd | C66 | ND-AzTtp       | 46  | 7   | 42  | Y | 9%    |
| Pd | C11 | ND-DUqr43      | 261 | 44  | 248 | Y | 5%    |
| Pd | C12 | ND-DUqr44      | 127 | 55  | 120 | Y | 6%    |
| Pd | C13 | ND-DUqr45      | 133 | 55  | 143 | Y | 7%    |
| Pd | C22 | ND-DUqr46      | 252 | 43  | 240 | Y | 5%    |
| Pd | C33 | ND-DUqr47      | 247 | 43  | 215 | Y | 15%   |
| Pd | C44 | ND-DUqr48      | 67  | 9   | 28  | Y | 140%  |
| Pd | C55 | ND-DUqr49      | 59  | 8   | 57  | Y | 3%    |
| Pd | C66 | ND-DUqr50      | 56  | 8   | 53  | Y | 5%    |
| Pd | C11 | diamond        | 219 | 59  | 41  | Y | 435%  |
| Pd | C12 | diamond        | 151 | 24  | 81  | Y | 86%   |
| Pd | C44 | diamond        | 37  | 22  | -28 | Y | 231%  |
| Pt | C11 | ND-cGAS2LRJaQh | 231 | 106 | 410 | Y | 44%   |
| Pt | C12 | ND-cGAS2LRJaQh | 182 | 90  | 103 | Y | 77%   |
| Pt | C13 | ND-cGAS2LRJaQh | 163 | 103 | 176 | Y | 8%    |
| Pt | C22 | ND-cGAS2LRJaQh | 216 | 101 | 410 | Y | 47%   |
| Pt | C33 | ND-cGAS2LRJaQh | 243 | 86  | 474 | Y | 49%   |
| Pt | C44 | ND-cGAS2LRJaQh | 88  | 15  | 6   | Y | 1363% |
| Pt | C55 | ND-cGAS2LRJaQh | 73  | 38  | 112 | Y | 35%   |
| Pt | C66 | ND-cGAS2LRJaQh | 94  | 16  | 111 | Y | 15%   |
| Pt | C11 | ND-5COO2H3     | 231 | 30  | 408 | Y | 43%   |
| Pt | C12 | ND-5COO2H4     | 141 | 36  | 185 | Y | 24%   |
| Pt | C13 | ND-5COO2H5     | 128 | 31  | 176 | Y | 27%   |
| Pt | C22 | ND-5COO2H6     | 231 | 30  | 409 | Y | 43%   |
| Pt | C33 | ND-5COO2H7     | 317 | 56  | 327 | Y | 3%    |
| Pt | C44 | ND-5COO2H8     | 58  | 3   | 111 | Y | 48%   |



|    |     |             |       |     |     |   |       |
|----|-----|-------------|-------|-----|-----|---|-------|
| Pt | C55 | ND-5COO2H9  | 58    | 3   | 3   | Y | 1840% |
| Pt | C66 | ND-5COO2H10 | 45    | 3   | 2   | Y | 2155% |
| Pt | C11 | ND-C9BvrCu  | -185  | 983 | 178 | Y | 204%  |
| Pt | C12 | ND-C9BvrCu  | -383  | 104 | 270 | Y | 242%  |
| Pt | C44 | ND-C9BvrCu  | 54    | 18  | 146 | Y | 63%   |
| Re | C11 | MP-1186901  | -4224 | 428 | 104 | Y | 4161% |
| Re | C12 | MP-1186901  | 5284  | 413 | 73  | Y | 7138% |
| Re | C13 | MP-1186901  | 491   | 136 | 73  | Y | 572%  |
| Re | C22 | MP-1186901  | -4238 | 429 | 104 | Y | 4175% |
| Re | C33 | MP-1186901  | 621   | 145 | 104 | Y | 497%  |
| Re | C44 | MP-1186901  | -2678 | 242 | 32  | Y | 8467% |
| Re | C55 | MP-1186901  | -2700 | 240 | 32  | Y | 8537% |
| Re | C66 | MP-1186901  | 50    | 21  | 32  | Y | 55%   |
| Re | C11 | MP-975065   | 894   | 96  | 597 | Y | 50%   |
| Re | C12 | MP-975065   | 652   | 119 | 278 | Y | 134%  |
| Re | C13 | MP-975065   | 642   | 121 | 215 | Y | 199%  |
| Re | C22 | MP-975065   | 873   | 117 | 597 | Y | 46%   |
| Re | C33 | MP-975065   | 884   | 116 | 670 | Y | 32%   |
| Re | C44 | MP-975065   | 83    | 4   | 151 | Y | 45%   |
| Re | C55 | MP-975065   | 74    | 2   | 151 | Y | 51%   |
| Re | C66 | MP-975065   | 80    | 1   | 160 | Y | 50%   |
| Re | C11 | MP-8642     | 925   | 114 | 560 | Y | 65%   |
| Re | C12 | MP-8642     | 702   | 122 | 265 | Y | 165%  |
| Re | C44 | MP-8642     | 79    | 2   | 218 | Y | 64%   |
| Re | C11 | sc          | 194   | 13  | 188 | Y | 3%    |
| Re | C12 | sc          | 61    | 80  | 305 | Y | 80%   |
| Re | C44 | sc          | 2     | 11  | -24 | Y | 110%  |
| Sb | C11 | MP-10630    | 59    | 45  | 60  | Y | 1%    |
| Sb | C12 | MP-10630    | 62    | 43  | 60  | Y | 3%    |
| Sb | C13 | MP-10630    | 78    | 33  | 58  | Y | 34%   |
| Sb | C22 | MP-10630    | 183   | 67  | 50  | Y | 266%  |
| Sb | C33 | MP-10630    | 72    | 38  | 53  | Y | 35%   |
| Sb | C44 | MP-10630    | 1     | 2   | -3  | Y | 130%  |
| Sb | C55 | MP-10630    | 1     | 3   | -5  | Y | 122%  |
| Sb | C66 | MP-10630    | 1     | 5   | -6  | Y | 120%  |
| Sb | C11 | MP-1179605  | 23    | 33  | 78  | Y | 71%   |
| Sb | C12 | MP-1179605  | -1    | 8   | 35  | Y | 104%  |
| Sb | C13 | MP-1179605  | -2    | 29  | 38  | Y | 105%  |
| Sb | C22 | MP-1179605  | -17   | 34  | 120 | Y | 114%  |
| Sb | C33 | MP-1179605  | -25   | 37  | 78  | Y | 132%  |
| Sb | C44 | MP-1179605  | -32   | 52  | 2   | Y | 1695% |
| Sb | C55 | MP-1179605  | 2     | 25  | 1   | Y | 120%  |
| Sb | C66 | MP-1179605  | 2     | 3   | 46  | Y | 96%   |
| Sb | C11 | MP-133      | 6     | 64  | 144 | Y | 96%   |
| Sb | C12 | MP-133      | -7    | 3   | 13  | Y | 153%  |
| Sb | C44 | MP-133      | -75   | 129 | 14  | Y | 638%  |

|    |     |            |     |     |     |   |      |
|----|-----|------------|-----|-----|-----|---|------|
| Sb | C11 | MP-7761    | 117 | 43  | 84  | Y | 40%  |
| Sb | C12 | MP-7761    | 92  | 35  | 56  | Y | 64%  |
| Sb | C44 | MP-7761    | 14  | 4   | 20  | Y | 28%  |
| Sr | C11 | MP-1187073 | 26  | 2   |     | Y |      |
| Sr | C12 | MP-1187073 | 5   | 2   |     | Y |      |
| Sr | C13 | MP-1187073 | 4   | 2   |     | Y |      |
| Sr | C22 | MP-1187073 | 19  | 4   |     | Y |      |
| Sr | C33 | MP-1187073 | 20  | 4   |     | Y |      |
| Sr | C44 | MP-1187073 | 3   | 3   |     | Y |      |
| Sr | C55 | MP-1187073 | 5   | 1   |     | Y |      |
| Sr | C66 | MP-1187073 | 5   | 1   |     | Y |      |
| Sr | C11 | MP-139     | 18  | 5   | 20  | Y | 10%  |
| Sr | C12 | MP-139     | 13  | 3   | 9   | Y | 44%  |
| Sr | C13 | MP-139     | 4   | 2   | 5   | Y | 28%  |
| Sr | C22 | MP-139     | 19  | 3   | 20  | Y | 7%   |
| Sr | C33 | MP-139     | 28  | 2   | 26  | Y | 7%   |
| Sr | C44 | MP-139     | 5   | 1   | 5   | Y | 4%   |
| Sr | C55 | MP-139     | 5   | 1   | 5   | Y | 2%   |
| Sr | C66 | MP-139     | 3   | 3   | 6   | Y | 55%  |
| Sr | C11 | MP-95      | 36  | 2   | 14  | Y | 157% |
| Sr | C12 | MP-95      | 7   | 2   | 11  | Y | 33%  |
| Sr | C44 | MP-95      | 10  | 0   | 14  | Y | 29%  |
| Sr | C11 | MP-1179325 | -6  | 65  | 104 | Y | 105% |
| Sr | C12 | MP-1179325 | -14 | 30  | 73  | Y | 119% |
| Sr | C13 | MP-1179325 | -14 | 30  | 73  | Y | 119% |
| Sr | C22 | MP-1179325 | 19  | 4   | 104 | Y | 82%  |
| Sr | C33 | MP-1179325 | 19  | 4   | 104 | Y | 82%  |
| Sr | C44 | MP-1179325 | 3   | 2   | 32  | Y | 91%  |
| Sr | C55 | MP-1179325 | 3   | 1   | 32  | Y | 92%  |
| Sr | C66 | MP-1179325 | 3   | 1   | 32  | Y | 92%  |
| Ti | C11 | MP-72      | -43 | 514 | 196 | Y | 122% |
| Ti | C12 | MP-72      | 278 | 178 | 83  | Y | 235% |
| Ti | C13 | MP-72      | 334 | 298 | 52  | Y | 542% |
| Ti | C22 | MP-72      | 224 | 60  | 196 | Y | 14%  |
| Ti | C33 | MP-72      | 139 | 266 | 251 | Y | 45%  |
| Ti | C44 | MP-72      | 16  | 8   | 52  | Y | 69%  |
| Ti | C55 | MP-72      | 16  | 8   | 52  | Y | 69%  |
| Ti | C66 | MP-72      | 32  | 11  | 56  | Y | 42%  |
| Ti | C11 | MP-6985    | 218 | 76  | 123 | Y | 77%  |
| Ti | C12 | MP-6985    | 188 | 54  | 99  | Y | 89%  |
| Ti | C44 | MP-6985    | 84  | 8   | 55  | Y | 53%  |
| Ti | C11 | MP-73      | 175 | 16  | 70  | Y | 150% |
| Ti | C12 | MP-73      | 112 | 34  | 123 | Y | 9%   |
| Ti | C44 | MP-73      | 21  | 9   | 39  | Y | 47%  |
| Ti | C11 | sc         | 53  | 19  |     | Y |      |
| Ti | C12 | sc         | 816 | 120 |     | Y |      |
| Ti | C44 | sc         | -22 | 70  |     | Y |      |
| Zn | C11 | MP-1187812 | 116 | 16  | 113 | Y | 2%   |
| Zn | C12 | MP-1187812 | 75  | 11  | 64  | Y | 17%  |
| Zn | C13 | MP-1187812 | 77  | 8   | 64  | Y | 20%  |

|    |     |              |     |    |     |   |      |
|----|-----|--------------|-----|----|-----|---|------|
| Zn | C22 | MP-1187812   | 114 | 18 | 82  | Y | 39%  |
| Zn | C33 | MP-1187812   | 93  | 9  | 83  | Y | 12%  |
| Zn | C44 | MP-1187812   | 14  | 1  | 21  | Y | 34%  |
| Zn | C55 | MP-1187812   | 12  | 1  | 31  | Y | 60%  |
| Zn | C66 | MP-1187812   | 21  | 3  | 38  | Y | 46%  |
| Zn | C11 | ND-NPwQaO    | 103 | 29 | 98  | Y | 5%   |
| Zn | C12 | ND-NPwQaO    | 66  | 23 | 49  | Y | 35%  |
| Zn | C13 | ND-NPwQaO    | 69  | 22 | 59  | Y | 17%  |
| Zn | C22 | ND-NPwQaO    | 104 | 29 | 135 | Y | 23%  |
| Zn | C33 | ND-NPwQaO    | 100 | 30 | 126 | Y | 20%  |
| Zn | C44 | ND-NPwQaO    | 22  | 2  | 46  | Y | 52%  |
| Zn | C55 | ND-NPwQaO    | 21  | 2  | 19  | Y | 13%  |
| Zn | C66 | ND-NPwQaO    | 20  | 2  | 40  | Y | 50%  |
| Zn | C11 | ND-wLmvfrkiz | 94  | 13 | 9   | Y | 943% |
| Zn | C12 | ND-wLmvfrkiz | 58  | 12 | 90  | Y | 35%  |
| Zn | C13 | ND-wLmvfrkiz | 58  | 12 | 90  | Y | 35%  |
| Zn | C22 | ND-wLmvfrkiz | 92  | 13 | 9   | Y | 920% |
| Zn | C33 | ND-wLmvfrkiz | 92  | 13 | 9   | Y | 920% |
| Zn | C44 | ND-wLmvfrkiz | 16  | 1  | 4   | Y | 293% |
| Zn | C55 | ND-wLmvfrkiz | 14  | 1  | 4   | Y | 240% |
| Zn | C66 | ND-wLmvfrkiz | 14  | 1  | 4   | Y | 240% |
| Zn | C11 | diamond      | 113 | 20 | 21  | Y | 437% |
| Zn | C12 | diamond      | 65  | 30 | 27  | Y | 139% |
| Zn | C44 | diamond      | 12  | 8  | -18 | Y | 168% |
| Zr | C11 | MP-1077723   | 217 | 16 |     | Y |      |
| Zr | C12 | MP-1077723   | 118 | 15 |     | Y |      |
| Zr | C13 | MP-1077723   | 136 | 15 |     | Y |      |
| Zr | C22 | MP-1077723   | 234 | 16 |     | Y |      |
| Zr | C33 | MP-1077723   | 217 | 16 |     | Y |      |
| Zr | C44 | MP-1077723   | 23  | 1  |     | Y |      |
| Zr | C55 | MP-1077723   | 40  | 2  |     | Y |      |
| Zr | C66 | MP-1077723   | 23  | 1  |     | Y |      |
| Zr | C11 | MP-8635      | 187 | 13 | 119 | Y | 57%  |
| Zr | C12 | MP-8635      | 107 | 20 | 76  | Y | 41%  |
| Zr | C44 | MP-8635      | 25  | 3  | 51  | Y | 50%  |

**Table S8.** DNP and DFT Phases *Not* Explicitly included in the Training Dataset.

| Element | Structure ID | $E_{\text{coh, DNP}}$ | s.d   | $E_{\text{coh, DFT}}$ | $V_{\text{DNP}}$ | s.d.   | $V_{\text{DFT}}$ | atoms | Error $E_{\text{coh, DNP}}$ | Error $V_{\text{DNP}}$ |
|---------|--------------|-----------------------|-------|-----------------------|------------------|--------|------------------|-------|-----------------------------|------------------------|
| Ag      | bcc          | -2.636                | 0.003 | -2.638                | 18.02            | 0.09   | 17.92            | 2     | 0%                          | 1%                     |
| Ag      | diamond      | -1.882                | 0.009 | -1.881                | 29.57            | 0.844  | 29.73            | 8     | 0%                          | 1%                     |
| Ag      | sc           | -2.306                | 0.007 | -2.329                | 20.62            | 0.237  | 20.61            | 1     | 1%                          | 0%                     |
| Au      | MP-1238808   | -2.308                | 0.008 | -2.331                | 17.67            | 0.186  | 17.94            | 2     | 1%                          | 2%                     |
| Au      | diamond      | -3.184                | 0.007 | -3.175                | 17.68            | 0.181  | 17.94            | 8     | 0%                          | 1%                     |
| Co      | MP-54_S      | -6.170                | 0.018 | -6.195                | 10.33            | 0.315  | 10.79            | 2     | 0%                          | 4%                     |
| Co      | MP-102_S     | -6.160                | 0.059 | -13.195               | 10.12            | 0.062  | 10.47            | 2     | 53%                         | 3%                     |
| Co      | MP-1271679_S | -5.921                | 0.01  | -6.193                | 11.60            | 0.05   | 10.27            | 4     | 4%                          | 13%                    |
| Co      | MP-1193227_S | -6.011                | 0.009 | -6.065                | 11.17            | 0.093  | 10.72            | 28    | 1%                          | 4%                     |
| Co      | MP-1072089   | -5.986                | 0.066 | -5.675                | 11.23            | 0.523  | 10.84            | 6     | 5%                          | 4%                     |
| Co      | MP-1183710   | -6.173                | 0.016 | -5.987                | 10.16            | 0.067  | 10.25            | 4     | 3%                          | 1%                     |
| Co      | bcc          | -6.160                | 0.059 | -5.754                | 10.12            | 0.062  | 10.47            | 2     | 7%                          | 3%                     |
| Co      | sc_S         | -5.536                | 0.031 | -5.413                | 12.72            | 0.13   | 11.80            | 1     | 2%                          | 8%                     |
| Cu      | MP-989782    | -3.661                | 0.002 | -3.672                | 11.91            | 0.045  | 11.95            | 2     | 0%                          | 0%                     |
| Cu      | MP-1059259   | -3.529                | 0.009 | -3.538                | 12.56            | 0.035  | 12.54            | 2     | 0%                          | 0%                     |
| Cu      | MP-1056079   | -3.660                | 0.003 | -3.677                | 11.93            | 0.016  | 11.93            | 1     | 0%                          | 0%                     |
| Cu      | diamond      | -3.283                | 0.505 | -2.649                | 15.25            | 5.358  | 19.08            | 8     | 24%                         | 20%                    |
| Cu      | sc           | -3.237                | 0.021 | -3.212                | 14.10            | 0.107  | 13.90            | 1     | 1%                          | 1%                     |
| I       | diamond      | -1.420                | 0.053 | -1.029                | 67.18            | 3.058  | 60.03            | 8     | 38%                         | 12%                    |
| I       | fcc          | -1.213                | 0.184 | -1.094                | 39.30            | 12.188 | 35.04            | 4     | 11%                         | 12%                    |
| I       | sc           | -1.245                | 0.006 | -1.265                | 40.42            | 1.21   | 41.30            | 1     | 2%                          | 2%                     |
| Kr      | diamond      | -0.115                | 0.128 | -0.030                | 102.81           | 48.534 | 116.85           | 8     | 288%                        | 12%                    |
| Kr      | sc           | -0.144                | 0.139 | -0.039                | 106.05           | 39.021 | 77.325           | 1     | 272%                        | 37%                    |
| Li      | MP-10173     | -1.857                | 0.002 | -1.858                | 20.30            | 0.026  | 20.30            | 2     | 0%                          | 0%                     |
| Li      | MP-567337    | -1.859                | 0.002 | -1.857                | 20.40            | 0.071  | 20.33            | 8     | 0%                          | 0%                     |
| Li      | MP-1103107   | -1.859                | 0.002 | -1.857                | 19.79            | 0.463  | 20.29            | 12    | 0%                          | 2%                     |
| Li      | MP-604313    | -1.859                | 0.002 | -1.857                | 19.76            | 0.458  | 20.29            | 4     | 0%                          | 3%                     |
| Li      | diamond      | -1.838                | 0.003 | -1.340                | 20.58            | 0.355  | 26.08            | 8     | 37%                         | 21%                    |
| Li      | sc           | -1.732                | 0.006 | -1.742                | 20.00            | 0.583  | 20.38            | 1     | 1%                          | 2%                     |
| Mg      | MP-110       | -1.490                | 0.004 | -1.490                | 22.48            | 0.223  | 22.76            | 1     | 0%                          | 1%                     |
| Mg      | MP-1056351   | -1.490                | 0.004 | -1.490                | 22.48            | 0.223  | 22.76            | 1     | 0%                          | 1%                     |
| Mg      | MP-1055956   | -1.509                | 0.002 | -1.502                | 22.73            | 0.176  | 23.08            | 1     | 0%                          | 2%                     |
| Mg      | bcc          | -1.490                | 0.004 | -1.497                | 22.48            | 0.223  | 22.87            | 2     | 0%                          | 2%                     |
| Mg      | diamond      | -1.459                | 0.006 | -0.725                | 23.19            | 0.22   | 40.40            | 8     | 101%                        | 43%                    |
| Mg      | sc           | -1.169                | 0.017 | -1.143                | 27.45            | 0.364  | 27.40            | 1     | 2%                          | 0%                     |
| Nb      | diamond      | -9.505                | 0.082 | -9.483                | 18.35            | 0.369  | 18.04            | 8     | 0%                          | 2%                     |
| Ni      | MP-10257_S   | -4.864                | 0.01  | -4.871                | 10.81            | 0.024  | 10.88            | 2     | 0%                          | 1%                     |
| Ni      | MP-1246134   | -4.519                | 0.015 | -4.476                | 12.00            | 0.045  | 11.70            | 1     | 1%                          | 3%                     |
| Ni      | MP-1014111_S | -4.864                | 0.01  | -4.871                | 10.81            | 0.024  | 10.88            | 2     | 0%                          | 1%                     |
| Ni      | MP-1094136_S | -4.871                | 0.004 | -4.896                | 10.85            | 0.065  | 10.85            | 2     | 1%                          | 0%                     |
| Ni      | diamond      | -3.646                | 0.045 | -3.605                | 18.63            | 1.249  | 16.40            | 8     | 1%                          | 14%                    |
| Ni      | sc           | -4.323                | 0.013 | -4.177                | 12.71            | 0.232  | 12.50            | 1     | 3%                          | 2%                     |
| Os      | bcc          | -9.948                | 0.051 | -9.432                | 13.95            | 0.469  | 14.76            | 2     | 5%                          | 5%                     |
| Os      | diamond      | -8.929                | 0.878 | -9.067                | 18.98            | 3.234  | 21.30            | 8     | 2%                          | 11%                    |
| Os      | sc           | -9.260                | 0.064 | -8.803                | 16.34            | 0.328  | 16.72            | 1     | 5%                          | 2%                     |
| Pb      | MP-20745     | -3.451                | 0.007 | -3.447                | 31.37            | 0.242  | 31.58            | 2     | 0%                          | 1%                     |
| Pb      | MP-1102666   | -3.448                | 0.009 | -3.467                | 31.43            | 0.151  | 31.72            | 12    | 1%                          | 1%                     |

|    |              |        |       |        |       |       |       |         |       |     |
|----|--------------|--------|-------|--------|-------|-------|-------|---------|-------|-----|
| Pb | sc           | -3.262 | 0.014 | -3.250 | 35.31 | 0.784 | 34.28 | 1       | 0%    | 3%  |
| Pd | MP-1186427_S | -3.791 | 0.013 | -3.769 | 15.29 | 0.115 | 15.34 | 4       | 1%    | 0%  |
| Pd | bcc          | -3.710 | 0.032 | -3.742 | 15.23 | 0.229 | 15.39 | 2       | 1%    | 1%  |
| Pd | sc           | -3.315 | 0.019 | -3.269 | 17.49 | 0.077 | 17.77 | 1       | 1%    | 2%  |
| Pt | ND-5COO2H3_S | -5.871 | 0.027 | -5.863 | 15.67 | 0.108 | 14.96 | 2       | 0%    | 5%  |
| Pt | sc           | -5.468 | 0.081 | -5.429 | 17.90 | 0.643 | 18.01 | 1       | 1%    | 1%  |
| Re | diamond      | -9.901 | 0.975 | -9.265 | 17.74 | 3.834 | 22.35 | 8       | 7%    | 21% |
| Sb | MP-1179613   | -3.881 | 0     | -3.918 | 32.76 | 0.484 | 32.27 | 14      | 1%    | 2%  |
| Sb | MP-632286    | -3.893 | 0.005 | -3.947 | 30.03 | 0.307 | 30.04 | 2       | 1%    | 0%  |
| Sb | MP-567409    | -3.911 | 0.002 | -4.001 | 31.93 | 0.202 | 31.40 | 4       | 2%    | 2%  |
| Sb | MP-1179618   | -3.855 | 0.012 | -3.784 | 33.04 | 0.062 | 34.25 | 14      | 2%    | 4%  |
| Sb | MP-1236935   | -3.836 | 0.014 | -3.837 | 32.89 | 0.21  | 32.97 | 14      | 0%    | 0%  |
| Sb | MP-567144    | -3.757 | 0.017 | 0.135  | 35.58 | 2.327 | 36.11 | 4       | 2889% | 1%  |
| Sb | MP-80        | -3.753 | 0.014 | -3.730 | 27.66 | 0.249 | 27.29 | 2       | 1%    | 1%  |
| Sb | diamond      | -3.589 | 0.067 | -3.683 | 42.94 | 0.783 | 42.92 | 8       | 3%    | 0%  |
| Sr | MP-1056418   | -1.618 | 0.004 | -1.617 | 55.76 | 0.563 | 54.69 | 1       | 0%    | 2%  |
| Sr | MP-867202    | -1.618 | 0.004 | -1.615 | 55.77 | 0.552 | 54.77 | 4       | 0%    | 2%  |
| Sr | MP-567826    | -1.612 | 0.008 | -1.610 | 55.29 | 0.247 | 52.99 | 4       | 0%    | 4%  |
| Sr | MP-19858     | -1.365 | 0.019 | -1.386 | 59.79 | 1.184 | 54.50 | 1       | 2%    | 10% |
| Sr | MP-639774    | -1.210 | 0.016 | -1.218 | 61.80 | 0.425 | 55.56 | 1       | 1%    | 11% |
| Ti | MP-1245164   | -6.135 | 0.049 | -6.099 | 17.02 | 0.03  | 17.17 | 10<br>0 | 1%    | 1%  |
| Ti | MP-1245006   | -6.094 | 0.002 | -6.100 | 17.09 | 0.058 | 17.13 | 10<br>0 | 0%    | 0%  |
| Ti | MP-1245320   | -6.107 | 0.016 | -6.088 | 17.07 | 0.045 | 17.18 | 10<br>0 | 0%    | 1%  |
| Ti | MP-1244924_S | -6.095 | 0.003 | -6.102 | 17.10 | 0.067 | 17.15 | 10<br>0 | 0%    | 0%  |
| Ti | MP-1244924   | -6.095 | 0.003 | -6.102 | 17.10 | 0.067 | 17.15 | 10<br>0 | 0%    | 0%  |
| Ti | MP-1238818   | -5.920 | 0.016 | -5.896 | 32.30 | 0.073 | 34.58 | 6       | 0%    | 7%  |
| Ti | diamond      | -5.664 | 0.729 | -3.930 | 19.24 | 3.851 | 21.28 | 8       | 44%   | 10% |
| Zr | diamond      | -7.014 | 0.172 | -7.118 | 24.15 | 1.225 | 23.14 | 8       | 1%    | 4%  |
| Zr | sc           | -6.479 | 0.011 | -6.305 | 24.60 | 0.578 | 24.73 | 1       | 3%    | 1%  |

**Table S9.** Comparison of DNP and DFT Vacancy Energies  $E_{v, \text{DNP/DFT}}$  (eV) and per atom Volumes  $V_{\text{DNP/DFT}}$  ( $\text{\AA}^3/\text{atom}$ ) Not Explicitly included in the Training Dataset.

| Element | Structure ID | $V_{\text{DNP}}$ | s.d.<br>$V_{\text{DNP}}$ | $V_{\text{DFT}}$ | atoms | $E_{\text{INT, DNP}}$ | s.d.<br>$E_{\text{INT, DNP}}$ | $E_{\text{INT, DFT}}$ | $E_v$ Error (%) |
|---------|--------------|------------------|--------------------------|------------------|-------|-----------------------|-------------------------------|-----------------------|-----------------|
| Ag      | bcc          | 18.637           | 0.074                    | 18.582           | 15    | 0.586                 | 0.016                         | 0.754                 | 22%             |
| Ag      | diamond      | 20.045           | 0.261                    | 24.174           | 7     | -4.376                | 0.044                         | -1.902                | 130%            |
| Ag      | sc           | 22.009           | 1.463                    | 22.930           | 7     | -0.020                | 1.116                         | 0.691                 | 103%            |
| Au      | MP-1238808   | 18.580           | 0.087                    | 18.658           | 15    | 0.709                 | 0.037                         | 0.363                 | 95%             |
| Au      | diamond      | 17.915           | 0.138                    | 18.169           | 63    | 0.802                 | 0.417                         | 0.675                 | 19%             |
| Co      | MP-54_S      | 11.039           | 0.022                    | 10.678           | 15    | 1.661                 | 0.208                         | 4.802                 | 65%             |
| Co      | MP-1271679_S | 11.039           | 0.022                    | 10.678           | 15    | -2.076                | 0.132                         | 4.778                 | 143%            |
| Co      | MP-1193227_S | 10.683           | 0.399                    | 10.494           | 27    | -2.530                | 0.131                         | 3.906                 | 165%            |
| Co      | MP-1183710   | 10.536           | 0.249                    | 10.463           | 31    | 1.719                 | 0.322                         | 1.831                 | 6%              |
| Co      | bcc          | 11.117           | 0.052                    | 10.782           | 15    | 2.290                 | 0.963                         | 0.569                 | 302%            |
| Co      | sc_S         | 12.608           | 0.566                    | 12.774           | 7     | -1.207                | 1.815                         | 3.345                 | 136%            |
| Cu      | MP-1059259   | 12.167           | 0.020                    | 12.183           | 31    | -3.038                | 0.238                         | -3.379                | 10%             |
| Cu      | MP-1056079   | 13.056           | 0.127                    | 12.925           | 7     | 0.964                 | 0.034                         | 0.975                 | 1%              |
| Cu      | diamond      | 13.427           | 0.103                    | 15.845           | 7     | -1.252                | 3.514                         | -2.578                | 51%             |
| Cu      | sc           | 14.013           | 0.936                    | 15.148           | 7     | -0.744                | 1.458                         | 0.945                 | 179%            |
| I       | diamond      | 73.494           | 2.046                    | 72.491           | 7     | 0.219                 | 0.305                         | -1.087                | 120%            |
| I       | fcc          | 76.332           | 5.907                    | 60.860           | 31    | -6.319                | 5.763                         | -15.117               | 58%             |
| I       | sc           | 44.386           | 0.148                    | 43.721           | 7     | 0.384                 | 0.069                         | -0.528                | 173%            |
| Li      | MP-10173     | 20.793           | 0.341                    | 20.825           | 15    | 0.465                 | 0.013                         | 0.512                 | 9%              |
| Li      | MP-567337    | 21.370           | 0.120                    | 21.163           | 15    | 0.603                 | 0.025                         | 0.559                 | 8%              |
| Li      | MP-1103107   | 13.095           | 6.285                    | 12.237           | 13    | 16.586                | 18.179                        | 24.711                | 33%             |
| Li      | MP-604313    | 20.478           | 0.193                    | 20.763           | 31    | 0.608                 | 0.016                         | 0.599                 | 2%              |
| Li      | diamond      | 22.517           | 0.395                    | 22.468           | 7     | 0.576                 | 0.010                         | -1.769                | 133%            |
| Li      | sc           | 22.865           | 0.422                    | 22.880           | 7     | 0.487                 | 0.008                         | 0.608                 | 20%             |
| Nb      | diamond      | 19.460           | 0.129                    | 19.403           | 7     | 2.928                 | 0.190                         | 2.602                 | 13%             |
| Ni      | MP-10257_S   | 11.412           | 0.068                    | 11.343           | 15    | 1.333                 | 0.009                         | 1.301                 | 2%              |
| Ni      | MP-1246134   | 10.852           | 0.063                    | 10.786           | 7     | -2.464                | 0.069                         | -2.551                | 3%              |
| Ni      | MP-1014111_S | 11.413           | 0.068                    | 11.343           | 15    | 1.333                 | 0.009                         | 1.301                 | 2%              |
| Ni      | MP-1094136_S | 11.441           | 0.076                    | 11.325           | 15    | 1.393                 | 0.041                         | 1.591                 | 12%             |
| Ni      | diamond      | 12.104           | 0.119                    | 13.946           | 7     | -6.689                | 0.347                         | -2.723                | 146%            |
| Ni      | sc           | 13.193           | 0.613                    | 13.604           | 7     | 0.166                 | 1.796                         | 1.458                 | 89%             |
| Os      | bcc          | 14.481           | 0.012                    | 14.917           | 15    | -0.135                | 0.651                         | -10.054               | 99%             |
| Os      | diamond      | 15.545           | 0.341                    | 24.346           | 7     | -6.176                | 6.189                         | 3.162                 | 295%            |
| Pb      | MP-20745     | 33.001           | 0.368                    | 32.883           | 15    | 0.365                 | 0.141                         | 0.468                 | 22%             |
| Pb      | MP-1102666   | 33.619           | 0.269                    | 33.316           | 11    | 0.380                 | 0.104                         | 0.452                 | 16%             |
| Pb      | sc           | 39.591           | 1.197                    | 37.475           | 7     | 0.674                 | 0.022                         | 0.521                 | 29%             |
| Pd      | bcc          | 15.652           | 0.171                    | 15.967           | 15    | 0.831                 | 0.230                         | 1.269                 | 35%             |
| Pd      | sc           | 17.776           | 1.105                    | 19.498           | 7     | -0.507                | 1.674                         | 1.511                 | 134%            |
| Pt      | 2_5COO2H3_S  | 16.257           | 0.112                    | 16.239           | 15    | 1.014                 | 0.104                         | 0.160                 | 534%            |
| Pt      | sc           | 18.981           | 1.416                    | 19.798           | 7     | 0.798                 | 0.933                         | 2.032                 | 61%             |
| Re      | diamond      | 16.650           | 0.052                    | 19.269           | 7     | -2.432                | 6.789                         | -1.276                | 91%             |
| Sb      | MP-1179613   | 33.119           | 0.310                    | 34.605           | 13    | 0.678                 | 0.118                         | 0.744                 | 9%              |
| Sb      | MP-632286    | 32.546           | 0.095                    | 32.685           | 15    | 0.054                 | 0.126                         | 0.353                 | 85%             |
| Sb      | MP-567409    | 32.061           | 0.086                    | 32.225           | 31    | 0.259                 | 0.065                         | 1.316                 | 80%             |
| Sb      | MP-1179618   | 32.547           | 0.151                    | 34.128           | 13    | 0.038                 | 0.125                         | -1.177                | 103%            |
| Sb      | MP-1236935   | 32.313           | 0.089                    | 32.410           | 13    | -0.640                | 0.105                         | -1.188                | 46%             |

|    |            |        |       |        |    |         |       |        |       |
|----|------------|--------|-------|--------|----|---------|-------|--------|-------|
| Sb | MP-80      | 32.856 | 0.439 | 32.718 | 15 | -1.641  | 0.147 | -2.209 | 26%   |
| Sb | diamond    | 33.877 | 0.058 | 34.856 | 7  | -1.205  | 0.566 | -1.066 | 13%   |
| Sr | MP-1056418 | 59.264 | 1.844 | 58.069 | 7  | 0.882   | 0.017 | 0.904  | 2%    |
| Sr | MP-867202  | 56.795 | 0.175 | 56.318 | 31 | 0.878   | 0.026 | 1.168  | 25%   |
| Sr | MP-567826  | 56.972 | 0.763 | 56.636 | 7  | 0.333   | 0.017 | 0.356  | 6%    |
| Sr | MP-19858   | 56.976 | 0.766 | 56.620 | 7  | -1.398  | 0.078 | -1.211 | 15%   |
| Sr | MP-639774  | 55.301 | 0.238 | 53.982 | 7  | -2.811  | 0.059 | -2.759 | 2%    |
| Ti | MP-1238818 | 33.023 | 0.231 | 35.129 | 47 | 1.220   | 0.505 | 1.261  | 3%    |
| Ti | diamond    | 18.522 | 0.024 | 17.202 | 7  | -1.523  | 4.942 | -7.866 | 81%   |
| Zr | diamond    | 25.096 | 1.300 | 25.043 | 7  | -57.988 | 0.094 | 2.238  | 2691% |

The "S" denoted that considerations of spin were included in the calculation of the DFT structure as these lattices have a Total magnetization above 1.00  $\mu\text{B}/\text{f.u.}$ .

**Table S10.** Surface Energies Calculated by DNP and DFT (mJ/m<sup>2</sup>).

| Element | Lattice | Miller Index   | DNP Average | DNP Standard deviation | DFT <sup>4</sup> | Error |
|---------|---------|----------------|-------------|------------------------|------------------|-------|
| Ag      | fcc     | 100            | 899         | 40                     | 818              | 10%   |
| Ag      | fcc     | 110            | 901         | 52                     | 875              | 3%    |
| Ag      | fcc     | 111            | 808         | 24                     | 764              | 6%    |
| Al      | fcc     | 100            | 935         | 33                     | 906              | 3%    |
| Al      | fcc     | 110            | 1006        | 10                     | 977              | 3%    |
| Al      | fcc     | 111            | 863         | 49                     | 769              | 12%   |
| Au      | fcc     | 100            | 1061        | 64                     | 861              | 23%   |
| Au      | fcc     | 110            | 1071        | 86                     | 909              | 18%   |
| Au      | fcc     | 111            | 839         | 57                     | 710              | 18%   |
| Co      | hcp     | 0001           | 1885        | 185                    | 2108             | 11%   |
| Co      | hcp     | 10 $\bar{1}$ 0 | 2657        | 87                     | 2257             | 18%   |
| Co      | hcp     | 11 $\bar{2}$ 0 | 2344        | 197                    | 2462             | 5%    |
| Cu      | fcc     | 100            | 1486        | 22                     | 1470             | 1%    |
| Cu      | fcc     | 110            | 1588        | 83                     | 1561             | 2%    |
| Cu      | fcc     | 111            | 1321        | 7                      | 1339             | 1%    |
| Ge      | dc      | 100            | 1166        | 19                     | 1398             | 17%   |
| Ge      | dc      | 110            | 856         | 85                     | 1109             | 23%   |
| Ge      | dc      | 111            | 1582        | 199                    | 1190             | 33%   |
| Li      | bcc     | 100            | 456         | 13                     | 462              | 1%    |
| Li      | bcc     | 110            | 497         | 27                     | 501              | 1%    |
| Li      | bcc     | 111            | 542         | 21                     | 544              | 0%    |
| Mg      | hcp     | 0001           | 674         | 16                     | 510              | 32%   |
| Mg      | hcp     | 10 $\bar{1}$ 0 | 1098        | 73                     | 597              | 84%   |
| Mg      | hcp     | 11 $\bar{2}$ 0 | 880         | 17                     | 757              | 16%   |
| Mo      | bcc     | 100            | 3746        | 428                    | 3182             | 18%   |
| Mo      | bcc     | 110            | 3661        | 409                    | 2783             | 32%   |
| Mo      | bcc     | 111            | 3938        | 448                    | 2962             | 33%   |
| Nb      | bcc     | 100            | 3252        | 147                    | 2275             | 43%   |
| Nb      | bcc     | 110            | 2834        | 91                     | 2060             | 38%   |
| Nb      | bcc     | 111            | 3183        | 87                     | 2339             | 36%   |
| Ni      | fcc     | 100            | 2090        | 42                     | 2208             | 5%    |
| Ni      | fcc     | 110            | 2189        | 40                     | 2286             | 4%    |
| Ni      | fcc     | 111            | 1891        | 24                     | 1924             | 2%    |
| Os      | hcp     | 0001           | 2711        | 159                    | 2950             | 8%    |
| Os      | hcp     | 10 $\bar{1}$ 0 | 3467        | 948                    | 3398             | 2%    |
| Os      | hcp     | 11 $\bar{2}$ 0 | 2951        | 43                     | 3932             | 25%   |
| Pb      | fcc     | 100            | 282         | 35                     | 328              | 14%   |
| Pb      | fcc     | 110            | 353         | 32                     | 331              | 7%    |
| Pb      | fcc     | 111            | 224         | 72                     | 263              | 15%   |
| Pd      | fcc     | 100            | 1534        | 155                    | 1522             | 1%    |
| Pd      | fcc     | 110            | 1643        | 114                    | 1574             | 4%    |
| Pd      | fcc     | 111            | 1304        | 103                    | 1359             | 4%    |
| Pt      | fcc     | 100            | 1959        | 242                    | 1856             | 6%    |
| Pt      | fcc     | 110            | 2202        | 488                    | 1871             | 18%   |



|    |     |                |      |     |      |     |
|----|-----|----------------|------|-----|------|-----|
| Pt | fcc | 111            | 1854 | 142 | 1488 | 25% |
| Re | hcp | 0001           | 2385 | 144 | 2566 | 7%  |
| Re | hcp | 10 $\bar{1}$ 0 | 4347 | 44  | 2859 | 52% |
| Re | hcp | 11 $\bar{2}$ 0 | 3556 | 73  | 3075 | 16% |
| Sr | fcc | 100            | 322  | 1   | 341  | 5%  |
| Sr | fcc | 110            | 330  | 0   | 407  | 19% |
| Sr | fcc | 111            | 299  | 5   | 342  | 13% |
| Ti | hcp | 0001           | 1808 | 104 | 1975 | 8%  |
| Ti | hcp | 10 $\bar{1}$ 0 | 2052 | 142 | 2031 | 1%  |
| Ti | hcp | 11 $\bar{2}$ 0 | 1833 | 65  | 1887 | 3%  |
| Zn | hcp | 0001           | 576  | 74  | 334  | 73% |
| Zn | hcp | 10 $\bar{1}$ 0 | 915  | 43  | 707  | 29% |
| Zn | hcp | 11 $\bar{2}$ 0 | 748  | 43  | 921  | 19% |
| Zr | hcp | 0001           | 1669 | 78  | 1599 | 4%  |
| Zr | hcp | 10 $\bar{1}$ 0 | 2066 | 184 | 1660 | 24% |
| Zr | hcp | 11 $\bar{2}$ 0 | 1804 | 113 | 1648 | 9%  |

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