Testing the $r^2$SCAN density functional for the thermodynamic stability of solids with and without a van der Waals correction

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Figure S1: Comparison of calculated and experimental formation enthalpies for the 1015 compounds for (a) SCAN and SCAN+rVV10 (b) r²SCAN and r²SCAN + rVV10. Multiple points for the same compound and functional correspond to different sources of experimental formation enthalpy. The dashed diagonal line corresponds to the $\Delta H_{\text{calc}} = \Delta H_{\text{expt}}$ line of perfect agreement.
Figure S2: Relative error of the calculated formation enthalpy plotted against the experimental formation enthalpy. The dashed vertical lines correspond to the $\Delta H_{\text{calc}} = \Delta H_{\text{expt}}$ line of perfect agreement. For the relative errors, the range is limited to ±150%.
Figure S3: Average Magnetic moment of 157 magnetic compounds, the horizontal line is leveled with PBE magnetic moment to show the difference.

Figure S4: Comparison of Mean Errors for PBE, SCAN, SCAN+rVV10, r²SCAN, and r²SCAN+rVV10 with respect to experimental values for formation enthalpies of solids. The 1015 set is partitioned into subsets defined in the main text. The numbers in parentheses above each set of bars indicate the number of compounds in that subset.
Table S1: Comparison of approximate bandgaps (eV) to experiment.

| System   | Expt | SCAN | $r^2$SCAN | SCAN+rVV10 | $r^2$SCAN+rVV10 |
|----------|------|------|-----------|------------|----------------|
| Ag$_2$O  | 1.2  | 0.245| 0.261     | 0.228      | 0.244          |
| Ag$_2$S  | 0.95 | 0.63 | 0.713     | 0.64       | 0.651          |
| AgCl     | 3.25 | 1.346| 1.437     | 1.309      | 1.383          |
| AgI      | 2.869| 1.641| 1.808     | 1.61       | 1.727          |
| Al$_2$O$_3$ | 9.7  | 7.196| 7.237     | 7.137      | 7.17           |
| Al$_2$Se$_3$ | 3.1  | 2.502| 2.526     | 2.469      | 2.489          |
| AlAs     | 2.1  | 1.754| 1.812     | 1.728      | 1.762          |
| AlN      | 5.74 | 4.933| 4.946     | 4.915      | 4.906          |
| AlP      | 2.45 | 1.911| 1.952     | 1.888      | 1.888          |
| AlSb     | 1.62 | 1.382| 1.497     | 1.352      | 1.456          |
| As       | 1.2  | 0    | 0.546     | 0.514      | 0.497          |
| AsI$_3$  | 2.29 | 2.297| 2.441     | 2.356      | 2.42           |
| BaF$_2$  | 9.06 | 7.203| 7.288     | 7.057      | 7.109          |
| BaO      | 5.13 | 2.336| 2.41      | 2.353      | 2.38           |
| BaS      | 3.88 | 2.489| 2.525     | 2.508      | 2.478          |
| BAs      | 1.46 | 1.415| 1.404     | 2.508      | 2.478          |
| BaTe     | 3.4  | 1.915| 1.971     | 1.911      | 1.926          |
| BeO      | 10.48| 8.591| 8.57      | 8.506      | 8.499          |
| Bi       | 0.015| 0    | 0         | 0          | 0              |
| Bi$_2$Se$_3$ | 0.21 | 0.51 | 0.831     | 0.637      | 0.778          |
| Bi$_2$Te$_3$ | 0.145| 0.392| 0.857     | 0.579      | 0.836          |
| BiI$_3$  | 1.73 | 2.615| 2.814     | 2.61       | 2.787          |
| BN       | 8    | 4.804| 4.905     | 4.78       | 4.882          |

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| System | Expt | SCAN | r²SCAN | SCAN+rVV10 | r²SCAN+rVV10 |
|--------|------|------|--------|------------|--------------|
| BP     | 2    | 1.52 | 1.467  | 1.525      | 1.446        |
| CaB₆   | 4.5  | 0.014| 0      | 0          | 0            |
| CaF₂   | 10   | 7.944| 8.006  | 7.87       | 7.896        |
| CaI₂   | 5.98 | 4.051| 4.176  | 4.143      | 4.136        |
| CaO    | 7.7  | 4.148| 4.231  | 4.166      | 4.193        |
| CaS    | 5.8  | 2.816| 2.847  | 2.824      | 2.816        |
| CaSe   | 4.87 | 2.514| 2.535  | 2.541      | 2.534        |
| CaTe   | 4.07 | 1.926| 1.979  | 1.954      | 1.978        |
| CdCl₂  | 5.7  | 4.069| 4.196  | 4.06       | 4.135        |
| CdO    | 1.2  | 0    | 0.075  | 0          | 0            |
| CdS    | 2.4175 | 1.554| 1.631  | 1.51       | 1.568        |
| CdSe   | 1.714| 0.925| 1.044  | 0.891      | 0.981        |
| CdTe   | 1.517| 0.967| 1.171  | 0.925      | 1.128        |
| CeN    | 0.7  | 0    | 0      | 0          | 0            |
| CeO₂   | 2.68 | 2.222| 2.179  | 2.224      | 2.2          |
| CoO    | 0.47 | 0.192| 0.313  | 0.287      | 0.287        |
| CoSi   | 0.045| 0    | 0      | 0          | 0            |
| Cr₂O₃  | 1.68 | 2.004| 1.418  | 2.172      | 1.384        |
| CrO₂   | 0.23 | 0    | 0      | 0          | 0            |
| CrSi₂  | 0.35 | 0    | 0      | 0          | 0            |
| CsCl   | 8.1  | 5.447| 5.485  | 5.319      | 5.342        |
| CsF    | 10   | 6.1  | 6.122  | 5.972      | 6.002        |
| CsI    | 6.37 | 4.42 | 4.472  | 4.302      | 4.338        |
| Cu₂O   | 2.023| 0.81 | 0.781  | 0.799      | 0.78         |

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| System   | Expt | SCAN | r²SCAN | SCAN+rVV10 | r²SCAN+rVV10 |
|----------|------|------|--------|------------|--------------|
| Cu₂Se    | 1.23 | 0    | 0      | 0          | 0            |
| Cu₂Te    | 1.08 | 0    | 0      | 0          | 0            |
| CuCl     | 3.306| 0.899| 0.98   | 0.863      | 0.901        |
| CuI      | 3.07 | 1.559| 1.707  | 1.497      | 1.623        |
| EuO      | 1.122| 3.011| 3.164  | 0          | 3.111        |
| EuS      | 1.645| 2.309| 2.386  | 2.339      | 2.348        |
| FeI₂     | 5.15 | 0    | 0.607  | 0          | 0.578        |
| FeP₂     | 0.4  | 0.769| 0.666  | 0.762      | 0.666        |
| FeS₂     | 1.2  | 1.641| 1.333  | 1.535      | 1.317        |
| FeSi     | 0.1  | 0    | 0      | 0          | 0            |
| FeTe₂    | 0.46 | 0    | 0      | 0          | 0            |
| Ga₂O₃    | 4.54 | 2.884| 2.964  | 2.812      | 2.906        |
| Ga₂S₃    | 3.59 | 2.275| 2.337  | 2.253      | 2.318        |
| Ga₂Se₃   | 2.05 | 1.503| 1.605  | 1.498      | 1.589        |
| GaAs     | 1.42 | 0.669| 0.957  | 0.682      | 0.937        |
| GaN      | 3.24 | 2.221| 2.323  | 2.195      | 2.291        |
| GaP      | 2.22 | 1.824| 1.864  | 1.823      | 1.809        |
| GaS      | 2.5  | 1.985| 2.108  | 2.053      | 2.057        |
| GaSb     | 0.725| 0.008| 0.405  | 0          | 0.406        |
| GaSe     | 1.98 | 1.388| 1.543  | 1.391      | 1.517        |
| Ge       | 0.665| 0.138| 0.313  | 0.313      | 0.313        |
| GeI₂     | 1.5  | 2.198| 2.306  | 2.204      | 2.261        |
| GeO₂     | 5.56 | 2.283| 2.444  | 2.278      | 2.436        |
| GeS      | 1.58 | 1.321| 1.379  | 1.322      | 1.361        |

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| System     | Expt | SCAN  | r^2SCAN | SCAN+rVV10 | r^2SCAN+rVV10 |
|------------|------|-------|---------|------------|---------------|
| GeSe       | 1.1  | 1.005 | 1.122   | 1.048      | 1.085         |
| GeSe₂      | 2.38 | 1.897 | 2       | 1.934      | 1.958         |
| GeTe       | 0.84 | 0.387 | 0.619   | 0.534      | 0.597         |
| I          | 1.3  | 1.194 | 1.248   | 1.233      | 1.233         |
| InAs       | 0.356| 0     | 0.094   | 0          | 0.078         |
| InN        | 2.4  | 0.015 | 0.086   | 0.028      | 0             |
| InS        | 1.86 | 1.797 | 1.821   | 1.721      | 1.805         |
| InSb       | 0.17 | 0     | 0.044   | 0          | 0             |
| InSe       | 1.187| 0.775 | 0.948   | 0.778      | 0.912         |
| K₂S        | 2.1  | 2.72  | 2.774   | 2.646      | 2.64          |
| K₂Se       | 1.8  | 2.494 | 2.565   | 2.416      | 2.454         |
| K₃Sb       | 1    | 0.761 | 0.817   | 0.712      | 0.752         |
| KCl        | 8.5  | 5.83  | 5.864   | 5.827      | 5.735         |
| KF         | 10.9 | 6.899 | 6.946   | 6.928      | 6.819         |
| KI         | 6.17 | 4.559 | 4.601   | 4.448      | 4.469         |
| Li₃Sb      | 1    | 1.056 | 1.185   | 1.088      | 1.151         |
| LiCl       | 9.33 | 7.483 | 7.519   | 7.565      | 7.558         |
| LiF        | 13.105| 10.643| 10.705  | 10.554     | 10.722        |
| LiI        | 6    | 5.083 | 5.169   | 5.01       | 5.038         |
| Mg₂Ge      | 0.532| 0.359 | 0.454   | 0.355      | 0.415         |
| Mg₂Pb      | 0.041| 0     | 0.271   | 0          | 0.24          |
| Mg₂Si      | 0.6  | 0.429 | 0.456   | 0.429      | 0.42          |
| MgF₂       | 11.8 | 8.096 | 8.147   | 7.998      | 8.044         |
| MgO        | 7.77 | 5.753 | 5.761   | 5.702      | 5.701         |

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| System | Expt | SCAN | \(r^2\)SCAN | SCAN+rVV10 | \(r^2\)SCAN+rVV10 |
|--------|------|------|-------------|------------|-------------------|
| MgSe   | 5.6  | 3.345| 3.366       | 3.287      | 3.296             |
| MgTe   | 4.7  | 3.079| 3.162       | 3.03       | 3.103             |
| MnF\(_2\) | 10.05| 1.623| 1.828       | 1.639      | 1.751             |
| MnI\(_2\) | 4.04 | 2.048| 2.146       | 2.114      | 2.109             |
| MnO    | 3.7  | 0    | 0           | 0          | 0                 |
| MnS    | 6.2  | 0.768| 0.928       | 0.894      | 0.927             |
| MnSe   | 1.8  | 0.834| 0.992       | 0.816      | 0.956             |
| MnTe   | 1.25 | 0    | 0           | 0          | 0                 |
| MoS\(_2\) | 1.07 | 1.207| 1.216       | 1.077      | 1.216             |
| Na\(_2\)S | 2.4 | 3.103| 3.157       | 3.039      | 3.098             |
| Na\(_2\)Se | 2 | 2.656| 2.727       | 2.588      | 2.623             |
| Na\(_2\)Te | 2.3 | 2.612| 2.724       | 2.579      | 2.625             |
| Na\(_3\)Sb | 1.1 | 0.949| 1.019       | 0.91       | 0.963             |
| NaCl   | 8.97 | 6.065| 6.047       | 5.906      | 6.027             |
| NaF    | 10.5 | 7.371| 7.442       | 7.22       | 7.329             |
| NaI    | 5.89 | 4.443| 4.479       | 4.368      | 4.425             |
| NiO    | 3.7  | 0.731| 0.779       | 0.927      | 0.777             |
| NiS    | 0.12 | 0    | 0           | 0          | 0                 |
| PbO    | 1.936| 1.359| 1.813       | 1.567      | 1.757             |
| PbO\(_2\) | 1.7 | 0    | 0           | 0.037      | 0                 |
| PbS    | 0.41 | 0.619| 0.802       | 0.716      | 0.767             |
| PbSe   | 0.27 | 0.555| 0.695       | 0.594      | 0.644             |
| PdO    | 1.5  | 0    | 0           | 0          | 0                 |
| PrO\(_2\) | 0.66 | 0    | 0           | 0          | 0                 |

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Table S1 – continued from previous page

| System | Expt | SCAN | r²SCAN | SCAN+rVV10 | r²SCAN+rVV10 |
|--------|------|------|--------|------------|--------------|
| PtS    | 0.8  | 0.888| 0.71   | 0.752      | 0.71         |
| PtS₂   | 0.75 | 1.343| 1.237  | 1.323      | 1.221        |
| RbCl   | 8.29 | 5.538| 5.579  | 5.411      | 5.436        |
| RbF    | 10.4 | 6.36 | 6.392  | 6.235      | 6.358        |
| RbI    | 5.83 | 4.415| 4.471  | 4.422      | 4.348        |
| ReSi₂  | 0.12 | 0    | 0      | 0          | 0            |
| S      | 3.82 | 2.745| 2.681  | 2.669      | 2.669        |
| Sb     | 0.1  | 0    | 0      | 0          | 0            |
| Sb₂Te₃ | 0.3  | 0.11 | 0.449  | 0.277      | 0.439        |
| Sbl₃   | 2.22 | 2.215| 2.346  | 2.237      | 2.317        |
| ScN    | 2.6  | 0.322| 0.394  | 0.354      | 0.354        |
| Se     | 1.75 | 1.372| 1.425  | 1.408      | 1.407        |
| Si     | 1.12 | 0.827| 0.787  | 0.767      | 0.748        |
| SiO₂   | 11   | 6.473| 6.538  | 6.379      | 6.411        |
| SmS    | 0.22 | 0    | 0      | 0          | 0            |
| SnI₂   | 2.4  | 1.903| 1.964  | 1.902      | 1.941        |
| SnO₂   | 2.7  | 1.679| 1.767  | 1.642      | 1.742        |
| SnS    | 1.08 | 1.075| 1.206  | 1.167      | 1.173        |
| SnS₂   | 2.07 | 1.855| 1.932  | 1.881      | 1.889        |
| SnSe   | 0.91 | 0.887| 1.095  | 1.006      | 1.062        |
| SnSe₂  | 1.03 | 0.933| 1.014  | 0.95       | 0.992        |
| SnTe   | 0.18 | 0.271| 0.149  | 0          | 0.13         |
| SrO    | 5.77 | 3.728| 3.785  | 3.719      | 3.747        |
| SrS    | 4.76 | 2.888| 2.93   | 2.91       | 2.873        |

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| System  | Expt | SCAN | r^2SCAN | SCAN+rVV10 | r^2SCAN+rVV10 |
|--------|------|------|---------|------------|---------------|
| SrSe   | 4.42 | 2.641| 2.693   | 2.646      | 2.609         |
| TaN    | 2.3  | 0    | 0       | 0          | 0             |
| TaS2   | 0.1  | 0    | 0       | 0          | 0             |
| TbO2   | 0.5  | 0    | 0       | 0          | 0             |
| Te     | 0.332| 0.531| 0.71    | 0.709      | 0.696         |
| ThO2   | 4.625| 4.859| 4.961   | 4.876      | 4.886         |
| Ti2O3  | 0.02 | 0    | 0       | 0          | 0             |
| TiO2   | 3    | 2.556| 2.572   | 2.541      | 2.572         |
| TiS2   | 1.24 | 0.23 | 0.31    | 0.272      | 0.271         |
| Tl2Te3 | 0.7  | 0.706| 0.89    | 0.762      | 0.86          |
| TICl   | 3.56 | 2.712| 2.788   | 2.707      | 2.709         |
| TII    | 2.67 | 2.355| 2.477   | 2.386      | 2.409         |
| TlSe   | 0.73 | 0.391| 0.446   | 0.41       | 0.422         |
| V2O3   | 0.1  | 0    | 0       | 0          | 0             |
| VO     | 0.3  | 0    | 0       | 0          | 0             |
| WS2    | 1.1  | 0    | 1.423   | 1.411      | 1.407         |
| YN     | 1.9  | 0.576| 0.62    | 0.621      | 0.62          |
| ZnI2   | 4.53 | 2.071| 2.194   | 2.102      | 2.162         |
| ZnO    | 3.35 | 1.151| 1.252   | 1.138      | 1.195         |
| ZnS    | 3.87 | 2.704| 2.744   | 2.653      | 2.672         |
| ZnSe   | 2.67 | 1.8  | 1.893   | 1.771      | 1.84          |
| ZnTe   | 2.25 | 1.598| 1.797   | 1.534      | 1.774         |
| ZrC    | 0.6  | 0    | 0       | 0          | 0             |
| ZrS2   | 1.68 | 1.314| 1.417   | 1.388      | 1.383         |