# Supplemental Information
# Reworking the *Tao–Mo* exchange-correlation functional: I. Reconsideration and Simplification

H. Francisco
*Quantum Theory Project, Dept. of Physics, University of Florida, Gainesville FL 32611*

A.C. Cancio
*Center for Computational Nanoscience, Dept. of Physics and Astronomy, Ball State University, Muncie IN 47306*

S.B. Trickey
*Quantum Theory Project, Dept. of Physics and Dept. of Chemistry, University of Florida, Gainesville FL 32611**

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We provide detailed equations for the *rreg* TM C functional, information on the *v1-sreg* TM version of our simplified X functional; a careful derivation of the gradient expansion of *sreg*TM exchange energy and how to satisfy the correct gradient expansion; lastly a system-by-system tabulation of the numerical results, including *v1-sreg*TM and *v3-sreg*TM, testing against standard molecular and crystalline system data sets.

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* francisco.hector@ufl.edu; trickey@ufl.edu

## I. CORRELATION FUNCTIONAL DETAILS

The *rreg* C energy per particle is given by

$$\epsilon_c^{rregTM} := \epsilon_c^0 f_{c1}(\alpha) + \epsilon_c^1 f_{c2}(\alpha) \ ., \tag{1}$$

The interpolation functions $f_{c1}$, $f_{c2}$ are defined below.

Quantities used in the various contributions are defined as

$$\zeta := (n_\uparrow - n_\downarrow)/(n_\uparrow + n_\downarrow) \tag{2}$$

and

$$\xi := \nabla\zeta/2(3\pi^2)^{2/3} \ . \tag{3}$$

Here $\sigma$ is the spin label, $\sigma =\uparrow$ or $\sigma =\downarrow$, and $n_\sigma = \sum_i |\varphi_{i\sigma}|^2$ (assuming integer occupation for simplicity).

The correlation energy per particle ingredients are

$$\epsilon_c^0 := (\epsilon_c^{LDA0} \ + \ H_0^{SCAN})G_c(\zeta) \tag{4}$$

and

$$\epsilon_c^1 := \epsilon_c^{LSDA1} \ + \ H_1^{PBE} \ . \tag{5}$$

Here $\epsilon_c^{LSDA1}$ is the PW92 local spin density approximation (LSDA) correlation energy density [1] and $H_1^{PBE}$ is

$$H_1^{PBE} = \gamma\phi^3 \ ln[1 + w_1(1 - g_1(At^2))] \ . \tag{6}$$

Definitions of the quantities involved are

$$t = (3\pi^2/16)^{1/3} s/\phi r_s^{1/2} \tag{7}$$
$$A = \beta(r_s)/(\gamma w_1) \tag{8}$$
$$w_1 = \exp[-\epsilon_c^{LSDA1}/(\gamma\phi^3)] - 1 \tag{9}$$
$$g_1(At^2) = 1/(1 + At^2 + A^2t^4) \tag{10}$$
$$\beta(r_s) = 0.066725(1 + 0.1r_s)/(1 + 0.1778r_s) \tag{11}$$
$$\phi(\zeta) = [(1 + \zeta)^{2/3} + (1 - \zeta)^{2/3}]/2 \ . \tag{12}$$

As usual, the local Wigner-Seitz radius is a function of the density $n(\mathbf{r})$,

$$r_s(\mathbf{r}) = (4\pi n(\mathbf{r})/3)^{-1/3} \ . \tag{13}$$

Also $\gamma = 0.031091$.

In Eq. 4, $\epsilon_c^{LDA0} G_c(\zeta)$ is the local correlation energy density form from the SCAN functional [2, 3]

$$\epsilon_c^{LDA0} = \frac{-b_{1c}}{1 + b_{2c} r_s^{1/2} + b_{3c} r_s} \ , \tag{14}$$

and

$$\begin{aligned} G_c(\zeta) &= \{1 - 2.3631(d_x(\zeta) - 1)\}(1 - \zeta^{12}) \\ d_x(\zeta) &= [(1+\zeta)^{4/3} + (1-\zeta)^{4/3}]/2 \ , \end{aligned} \tag{15}$$

and

$$H_0^{SCAN} = b_{1c} \ ln[1 + w_0(1 - g_\infty(\zeta = 0, s))] \ . \tag{16}$$

The various quantities are

$$w_0 := \exp[-\epsilon_c^{LDA0}/b_{1c}] - 1 \tag{17}$$

$$g_\infty(\zeta, s)) := \lim_{r_s \to \infty} g_0(At^2) = 1/(1 + 4\chi_\infty s^2)^{1/4} \tag{18}$$

$$\chi_\infty(\zeta) := (3\pi^2/16)^{2/3} \beta(r_s \to \infty)\phi/[C_x(\zeta) - f_0] \tag{19}$$

$$C_x(\zeta) \ = \ (-3/4\pi)(9\pi/4)^{1/3} d_x(\zeta) \ . \tag{20}$$

$f_0 = -0.9$, at $\zeta = 0$, $\chi_\infty(\zeta = 0) = 0.128026$. The parameters are $b_{1c} = 0.0285764$, $b_{2c} = 0.0889$, and $b_{3c} = 0.125541$.

Finally, the interpolation functions $f_{c1}(\alpha)$ and $f_{c2}(\alpha)$ that appear in Eq. (1) are

$$f_{c2}(\alpha) = \frac{3[g(\alpha)]^3}{1 + [g(\alpha)]^3 + [g(\alpha)]^6}, \tag{21}$$

with

$$g(\alpha) = \frac{(1+\gamma_1)\alpha}{\gamma_1 + \alpha}, \quad \gamma_1 = 0.2, \tag{22}$$

and

$$f_{c1}(\alpha) = 1 - f_{c2}(\alpha) \ . \tag{23}$$

The quantity $\tilde{\epsilon}_c = max[\epsilon_c^{PBE}(n_\sigma, 0, \nabla n_\sigma, 0), \epsilon_c^{PBE}(n_\uparrow, n_\downarrow, \nabla n_\uparrow, \nabla n_\downarrow)]$, where $\epsilon_c^{PBE}$ is the PBE GGA correlation energy per particle [4].

In original TM, instead of the TPSS $C$ function

$$C(\zeta, \xi)^{TPSS} = \frac{0.53 + 0.87\zeta^2 + 0.50\zeta^4 + 2.26\zeta^6}{\{1 + \xi^2[(1+\zeta)^{-4/3} + (1-\zeta)^{-4/3}]/2\}^4}, \tag{24}$$

$C$ is given by

$$C(\zeta, \xi)^{TM} = \frac{0.10\zeta^2 + 0.32\zeta^4}{\{1 + \xi^2[(1+\zeta)^{-4/3} + (1-\zeta)^{-4/3}]/2\}^4}. \tag{25}$$

## II. ANALYSIS OF NEARLY UNIFORM ELECTRON GAS LIMIT OF *sreg*TM META-GGA FUNCTIONALS.

### A. General structure of TM in the nearly-uniform limit.

The slowly varying electron gas is defined by $p, |q| \ll 1$, with $p$ as defined in Eq. (5) of the text and $q := \nabla^2 n/4k_F^2 n$ ($k_F := (3\pi^2 n)^{1/3}$) is the reduced Laplacian of the density. In this regime $\alpha$ has the gradient expansion

$$\alpha \to 1 + \frac{20}{9}q - \frac{40}{27}p \, . \tag{26}$$

The homogeneous electron gas limit is the extreme case $p = q = 0$ and $\alpha = 1$.

From the definitions of $w$ Eq. (19) and $z_{rev}$, Eq. (27) of the main text, their homogeneous electron gas limits in terms of the regularization parameter $\epsilon_p$ are

$$z_0(\epsilon_p) := z_{rev}(p = 0, \alpha = 1) = \frac{\epsilon_p}{3 + \epsilon_p} \tag{27}$$

$$w_0(\epsilon_p) := w(z_0) = \frac{z_0^2 + 3z_0^3}{(1 + z_0^3)^2} \, . \tag{28}$$

For $\epsilon_p = 0.5$ these go to

$$z_{rev} \to z_0(0.5) = 1/7 \tag{29}$$

$$w \to w_0(0.5) = 0.02899 \, . \tag{30}$$

The essential structure of the TM enhancement factor $F_x$ is

$$F_x = wF_x^{DME} + (1 - w)F_x^{SC} \, . \tag{31}$$

Since the two limiting functionals for exchange (Eq. (7) and (17) of the main text) both tend to one in the homogeneous electron gas limit, namely

$$F_x^{SC} \to 1 \tag{32}$$

$$F_x^{DME} \to 1, \tag{33}$$

the limit of Eq. (31) becomes

$$F_x^{(0)} = w_0 + (1 - w_0) = 1 \tag{34}$$

irrespective of the value of $w_0$, and thus of $\epsilon_p$. Thus the homogeneous electron gas limit is correct for all variants of *sreg*TM exchange.

For the weakly varying case, $p, q \to 0$,, the X enhancement factor may be expressed as

$$F_x \sim 1 + F_x^{(2)} + F_x^{(4)} + \cdots \, . \tag{35}$$

Here (0) indicates the value for uniform density, (2) the second-order gradient expansion correction, i.e., the term linear in $p$ and $q$, and (4) is the correction for the fourth-order term in the gradient expansion, with terms proportional to $p^2$, $q^2$, and $pq$.

To get the second-order result, we need expansions for the quantities in Eq. (31). We start by simply proposing

gradient expansions for $w$, $F_x^{DME}$ and $F_x^{SC}$:

$$w \sim w_0 + w_p p + w_q q \tag{36}$$
$$F_x^{SC} \sim 1 + \delta_p^{SC} p + \delta_q^{SC} q \tag{37}$$
$$F_x^{DME} \sim 1 + \delta_p^{DME} p + \delta_q^{DME} q \tag{38}$$

It will not be necessary to evaluate $w_{p,q}$, but the others must be done. Substituting those three expressions into Eq. (31) and taking all terms to second order gives

$$\begin{aligned} F_x^{(2)} = &(w_p p + w_q q) + w_0(\delta_p^{DME} p + \delta_q^{DME} q) \\ &+ (1 - w_0)(\delta_p^{SC} p + \delta_q^{SC} q) - (w_p p + w_q q) \ . \end{aligned} \tag{39}$$

That has the simple form

$$F_x^{(2)} = \delta_p^{SC} p + \delta_q^{SC} q + w_0(\Delta_p p + \Delta_q q) \ , \tag{40}$$

in which we have defined

$$\Delta_p := \delta_p^{DME} - \delta_p^{SC} \tag{41}$$
$$\Delta_q := \delta_q^{DME} - \delta_q^{SC} \ . \tag{42}$$

It is important to observe that the structure of the various TM X functionals has the DME ("density matrix expansion") and SC ("slowly varying correction" per Ref. 5) contributions. Therefore we expect the desired quantity to be the gradient expansion for the SC term, since it is designed to return the correct one. That is, the error in our functional should be characterized by $\Delta_p$ and $\Delta_q$. Unfortunately, the SC itself has errors in the gradient expansion in sregTM, caused by a nonzero value of $z$ for $p, q = 0$. Since the desired gradient expansion correction is

$$F_x^{(2)} = \frac{10}{81} p \tag{43}$$

our error expression becomes

$$\delta F_x^{(2)} = (\delta_p^{SC} - 10/81)p + \delta_q^{SC} q + w_0(\Delta_p p + \Delta_q q). \tag{44}$$

Note that the magnitude of the error is of order $w_0$, which is a small number, and we expect an error of a few percent.

## B. Working out gradient expansion error

### 1. *The "SC" term*

The form for $F_x^{sc}$ is given in Eq. (17) of the main text. It depends upon $\tilde{q}$, which is designed to be a substitute for $q$, hence

$$\tilde{q} \to q \tag{45}$$

in the slowly-varying limit. Given this, the second-order term in the gradient expansion of Eq. (17) is

$$\frac{10}{81} p - \frac{73}{405} q \frac{3}{5} z_0 (1 - z_0) \tag{46}$$

which, after substitutions is

$$\delta^{SC} = \frac{10}{81}p - \frac{73}{225}\frac{\epsilon_p}{(3+\epsilon_p)^2}q, \tag{47}$$

or

$$\delta_p^{SC} = \frac{10}{81} \tag{48}$$

$$\delta_q^{SC} = -\frac{73}{225}\frac{\epsilon_p}{(3+\epsilon_p)^2}\ . \tag{49}$$

The latter coefficient reduces to -146/11025 or roughly 0.013 if $\epsilon_p = 0.5$, a factor of ten smaller than the exact coefficient 10/81. The second-order error Eq. (44) now is reduced to

$$\delta F_x^{(2)} = \delta_q^{SC} + w_0(\Delta_p p + \Delta_q q)\ . \tag{50}$$

### *2. The "DME" term*

Analysis of the contribution from this term is much harder. Begin with the definitions for $F_x^{DME}$, Eq. (7), $f$, Eq. (8), and $R$, Eq. (9) in the main text, along with the associated constants $\beta = 79.873$, $\lambda = 0.6866$ and auxiliary functions

$$y := (2\lambda - 1)^2 p \tag{51}$$

$$z_2 := 5p/3 \tag{52}$$

$$z_3 := z_2 + \alpha \tag{53}$$

$$z_4 := z_3 - 1 - z_2/9. \tag{54}$$

We have defined $z_4$ to make later analysis easier. The other three were defined at Eqs. (10), (11), and (12) of the main text.

Working backwards, the slowly varying limits of these are

$$y \to (2\lambda - 1)^2 p \tag{55}$$

$$z_2 \to \frac{5}{3}p \tag{56}$$

$$z_3 \to 1 + \frac{20}{9}q + \frac{5}{27}p \tag{57}$$

$$z_4 \to \frac{20}{9}q \tag{58}$$

and

$$R \sim 1 + 595(2\lambda - 1)^2\frac{p}{54} - \left(1 + \frac{20}{9}q + \frac{5}{27}p\right) + \left[3(\lambda^2 - \lambda + 1/2)\right]\frac{20}{9}q \tag{59}$$

or

$$\left[\frac{595}{54}(2\lambda - 1)^2 - \frac{5}{27}\right]p + \left[3(\lambda^2 - \lambda + 1/2) - 1\right]\frac{20}{9}q \tag{60}$$

Also

$$f \to 1 + \frac{70}{27}y \tag{61}$$

or

$$f \to 1 + \frac{70}{27}(2\lambda - 1)^2 p \tag{62}$$

so that

$$f^{-n} \to 1 - n\frac{70}{27}(2\lambda - 1)^2 p \tag{63}$$

Combined, these yield

$$F_x^{DME} \to 1 - 2\frac{70}{27}(2\lambda - 1)^2 p + \frac{7}{9}R \tag{64}$$

so that we get second-order gradient expansion coefficients that read

$$\begin{aligned} \delta_p^{DME} &= -\frac{140}{27}(2\lambda - 1)^2 \\ &\quad + \frac{7}{9}\left[\frac{595}{54}(2\lambda - 1)^2 - \frac{5}{27}\right] \end{aligned} \tag{65}$$

$$\delta_q^{DME} = \left[3(\lambda^2 - \lambda + 1/2) - 1\right]\frac{140}{81}\ . \tag{66}$$

With $\lambda = 0.6866$, these evaluate to $\delta_p^{DME} = 0.32739$ and $\delta_q^{DME} = -0.25155$.

### *3. Putting it all together*

Overall, for $\delta F_x^{(2)}$ from Eqs. 50, 41, 42, 49, 65 and 66 we get

$$\delta F_x^{(2)} = \delta_q^{SC} + w_0\left[\left(\delta_p^{DME} - \frac{10}{81}\right)p + \left(\delta_q^{DME} - \delta_q^{SC}\right)q\right]. \tag{67}$$

To evaluate these coefficients we used a python script to get

$$\delta F_x^{(2)} = \delta_p p + \delta_q q\ . \tag{68}$$

For the chosen value $\epsilon_p = 0.5$, the result is $\delta_p = 0.005912$ and $\delta_q = -0.020151$.

If one wishes, using a gauge invariant transformation of the term dependent on $q$ to one depending on $p$,

$$\delta_q q \to \delta_q p/3 \tag{69}$$

using, via integration by parts,

$$\int q e_x^{LDA} d^3r = \frac{1}{3}\int p e_x^{LDA} d^3r \tag{70}$$

where $e_x^{LDA} \sim n^{4/3}$ is LDA (Dirac) exchange energy density. This yields a final estimate of the gradient expansion error in *v2-sreg*TM of

$$\delta F_{x,v2}^{(2)} = (\delta_p + \delta_q/3)p = -0.000805p. \tag{71}$$

Fortunate error cancellation puts the result within 0.6% error of the correct value of 0.1235, in practice therefore not leading to the need for any meaningful correction.

The fortuitous cancellation of errors in *v2-sreg*TM between error arises from from the $z$-dependence of $F_x^{SC}$ and of

$w$. Noting that both terms are of course functions of $\epsilon_p$, we have an overall function of $\epsilon_p$, $\delta F_x^{(2)}(\epsilon_p)$ that is near a root for $\epsilon = 0.5$. A numerical search for this root returns:

$$\epsilon_p^{GE2} = 0.58568 \tag{72}$$

which then yields a fractional error in the second-order contribution to the exchange energy of $-2 \times 10^{-10}$.

Finally we note that for *v1-sreg*TM, there are changes to $z_{rev}$ only in $w$ and none in $F_x^{SC}$. Taking this into account sets $\delta_q^{SC}$ to zero everywhere and changes Eq. 67 to

$$\delta F_{x,v1}^{(2)} = w_0 \left[ \left( \delta_p^{DME} - \frac{10}{81} \right) p + \delta_q^{DME} q \right] \tag{73}$$

with the net result after integration by parts of

$$\delta F_{x,v1}^{(2)} = 0.003481 p. \tag{74}$$

This is still only a few percent off the correct answer, but we lack an obvious mechanism for enforcing exact compliance.

## III. *v1-sreg* TM X

Here we provide parametrization for the *v1-sreg*TM X functional and comparison of its performance with the *v2-sreg*TM X functional when used with both *rreg*TM and PBE correlation functionals.

TABLE I. Molecular test set results for the *v1-sreg*TM exchange functional combined with the *rreg*TM correlation functional for different values of $\epsilon_p$. Heat of formation errors in *kcal/mol*, bond length errors in $\mathring{A}$, and frequency errors in $cm^{-1}$.

| | | *v1-sreg*TM X + *rreg*TM C | | | | | | | *rreg*TM XC |
|---|---|---|---|---|---|---|---|---|---|
| | $\epsilon_p$ | 0.01 | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | |
| Heats of Formation | ME | 3.228 | 1.953 | 0.501 | -0.905 | -2.233 | -3.467 | -4.604 | **-3.790** |
| | MAE | 8.706 | 7.729 | 6.860 | 6.258 | 5.923 | 5.885 | 6.194 | **5.612** |
| Bonds | ME | 0.015 | 0.015 | 0.015 | 0.014 | 0.014 | 0.013 | 0.011 | **0.012** |
| | MAE | 0.018 | 0.017 | 0.017 | 0.016 | 0.016 | 0.015 | 0.014 | **0.014** |
| Frequencies | ME | -25.941 | -24.788 | -23.531 | -22.190 | -20.841 | -19.618 | -18.388 | **-21.011** |
| | MAE | 36.649 | 36.011 | 35.490 | 34.998 | 34.608 | 34.28 | 33.957 | **35.578** |

Table II gives the results for both *v1-sreg*TM X and *v2-sreg*TM X for the molecular test sets.

Table III gives the results for both *v1-sreg*TM X and *v2-sreg*TM X for the solid test sets.

Note that the use of *v1-sreg*TM X instead of *v2-sreg*TM X degrades bulk modulus performance for solids, but otherwise is comparable with the second variant *v2-sreg*TM X. Since, however, the second variant is simpler and slightly better in overall performance, we chose it.

## IV. MAGNETIZATION ENERGETICS

Table IV gives the saturation magnetic moment results for both *v1-sreg*TM X and *v2-sreg*TM X for the *3d* solids in comparison with other functionals.

Details follow in Tables V, VI, and VII.

TABLE II. Summary of molecular test set results for the *v1-sreg*TM and *v2-sreg*TM xchange functionals (both with $\epsilon_p = 0.5$) combined with the *rreg*TM correlation functional, as well as *v2-sreg*TM X with PBE C versus *rreg*TM X combined with PBE C, all compared with PBE XC and r$^2$SCAN XC. Heat of formation errors in $kcal/mol$, bond length errors in $\mathring{A}$, and frequency errors in $cm^{-1}$.

| | X<br>C | *rreg*TM<br>*rreg*TM | *v1-sreg*TM<br>*rreg*TM | *v2-sreg*TM<br>*rreg*TM | *v3-sreg*TM<br>*rreg*TM | *rreg*TM<br>*PBE* | *v2-sreg*TM<br>*PBE* | r$^2$SCAN<br>r$^2$SCAN | *PBE*<br>*PBE* |
|---|---|---|---|---|---|---|---|---|---|
| Heats of Formation | ME | -3.79 | -3.467 | -3.512 | -4.411 | -2.208 | -1.520 | -3.145 | -20.878 |
| | MAE | 5.612 | 5.885 | 5.895 | 6.128 | 5.452 | 5.354 | 4.488 | 21.385 |
| Bonds | ME | 0.012 | 0.013 | 0.013 | 0.011 | 0.008 | 0.008 | 0.005 | 0.018 |
| | MAE | 0.014 | 0.015 | 0.015 | 0.014 | 0.011 | 0.011 | 0.010 | 0.018 |
| Frequencies | ME | -21.011 | -19.618 | -19.275 | -18.354 | -4.667 | -2.865 | 11.336 | -33.781 |
| | MAE | 35.578 | 34.28 | 34.272 | 34.120 | 25.183 | 24.138 | 30.899 | 43.613 |

TABLE III. Comparison of solid system errors for DFA combinations as in Table II for four solid test sets. Equilibrium lattice constant errors in $\mathring{A}$, cohesive energy errors in $eV/atom$, bulk modulus errors in $GPa$, and Kohn-Sham band gap errors in $eV$.

| | X<br>C | *rreg*TM<br>*rreg*TM | *v1-sreg*TM<br>*rreg*TM | *v2-sreg*TM<br>*rreg*TM | *v3-sreg*TM<br>*rreg*TM | *rreg*TM<br>*PBE* | *v2-sreg*TM<br>*PBE* | r$^2$SCAN<br>r$^2$SCAN | *PBE*<br>*PBE* |
|---|---|---|---|---|---|---|---|---|---|
| Lattice constants | ME | 0.000 | 0.002 | 0.004 | 0.005 | -0.006 | -0.002 | 0.026 | 0.046 |
| | MAD | 0.029 | 0.030 | 0.031 | 0.031 | 0.028 | 0.029 | 0.037 | 0.053 |
| Cohesive energies | ME | 0.212 | 0.180 | 0.159 | 0.148 | 0.248 | 0.199 | -0.134 | -0.070 |
| | MAD | 0.251 | 0.232 | 0.216 | 0.210 | 0.288 | 0.251 | 0.238 | 0.252 |
| Bulk moduli | ME | 1.856 | 0.666 | 0.223 | 0.140 | 4.375 | 2.732 | 1.367 | -9.704 |
| | MAD | 6.740 | 6.811 | 6.602 | 6.450 | 7.200 | 6.542 | 5.963 | 11.022 |
| Band Gaps | ME | -1.52 | -1.54 | -1.53 | -1.52 | -1.42 | -1.44 | -1.20 | -1.69 |
| | MAD | 1.52 | 1.54 | 1.53 | 1.52 | 1.42 | 1.44 | 1.20 | 1.69 |

TABLE IV. Saturation magnetic moments in $\mu_B$ for some $3d$ solids with *v1-sreg*TM and *v2-sreg*TM X functionals (both with $\epsilon_p = 0.5$) combined with the *rreg*TM correlation functional, as well as *v2-sreg*TM X with PBE C versus *rreg*TM X combined with PBE C, all compared with PBE XC and r$^2$SCAN XC. "Exp." denotes the experimental saturation magnetization.

| | Exp. | X<br>C | *rreg*TM<br>*rreg*TM | *v1-sreg*TM<br>*rreg*TM | *v2-sreg*TM<br>*rreg*TM | *rreg*TM<br>*PBE* | *v2-sreg*TM<br>*PBE* | r$^2$SCAN<br>r$^2$SCAN | *PBE*<br>*PBE* |
|---|---|---|---|---|---|---|---|---|---|
| Fe | 2.22 | | 2.10 | 2.16 | 2.17 | 2.10 | 2.18 | 2.64 | 2.18 |
| Co | 1.72 | | 1.72 | 1.73 | 1.73 | 1.72 | 1.74 | 1.83 | 1.64 |
| Ni | 0.62 | | 0.68 | 0.66 | 0.66 | 0.68 | 0.66 | 0.72 | 0.63 |

TABLE V. Energy of bcc Fe and its saturation magnetic moments for the different functionals sorted in descending order. "Exp." denotes the experimental saturation magnetization.

| Functional | Energy<br>$eV$ | Magnetization<br>$\mu_B$ |
|---|---|---|
| Exp. | | 2.22 |
| PBE XC | -0.5293 | 2.18 |
| *rreg*TM X + PBE C | -0.6516 | 2.10 |
| *rreg*TM XC | -0.6535 | 2.10 |
| *v1-sreg*TM X + *rreg*TM C | -0.6653 | 2.16 |
| *v2-sreg*TM X + *rreg*TM C | -0.6751 | 2.17 |
| *v2-sreg*TM X + PBE C | -0.6770 | 2.18 |
| r$^2$SCAN XC | -1.2375 | 2.64 |

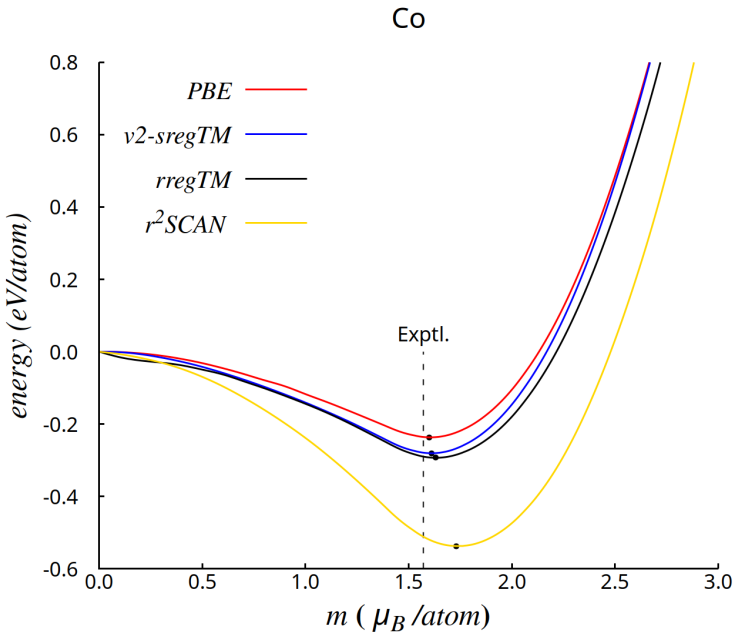


FIG. 1. Fixed spin moment energy for hcp Co using calculated equilibrium lattice parameter, on a per-atom basis for. Comparation of different functionals.

TABLE VI. As in Table V for fcc Co.

| Functional | Energy $eV$ | Magnetization $\mu_B$ |
|---|---|---|
| Exp. | | 1.72 |
| PBE XC | -0.2055 | 1.64 |
| *v1-sreg*TM X + *rreg*TM C | -0.2875 | 1.73 |
| *v2-sreg*TM X + *rreg*TM C | -0.2946 | 1.73 |
| *rreg*TM XC | -0.2996 | 1.72 |
| *v2-sreg*TM X + PBE C | -0.3032 | 1.74 |
| *reg*TM X + PBE C | -0.3082 | 1.72 |
| r$^2$SCAN XC | -0.5599 | 1.83 |

TABLE VII. As in Table V for fcc Ni.

| Functional | Energy $eV$ | Magnetization $\mu_B$ |
|---|---|---|
| Exp. | | 0.62 |
| PBE XC | -0.0583 | 0.63 |
| *v1-sreg*TM X +*rreg*TM C | -0.0805 | 0.66 |
| *v2-sreg*TM X + PBE C | -0.0811 | 0.66 |
| *v2-sreg*TM X + *rreg*TM C | -0.0814 | 0.66 |
| *rreg*TM XC | -0.0875 | 0.68 |
| *reg*TM X + PBE C | -0.0879 | 0.68 |
| r$^2$SCAN XC | -0.1187 | 0.72 |

TABLE VIII. As in Table V for hcp Co.

| Functional | Energy $eV$ | Magnetization $\mu_B$ |
|---|---|---|
| Exp. | | 1.57 |
| PBE XC | -0.2369 | 1.60 |
| *v2-sreg*TM X + *rreg*TM C | -0.2808 | 1.61 |
| *rreg*TM XC | -0.2934 | 1.63 |
| *reg*TM X + PBE C | -0.3002 | 1.63 |
| *v1-sreg*TM X + *rreg*TM C | -0.3052 | 1.63 |
| *v2-sreg*TM X + PBE C | -0.3164 | 1.64 |
| r$^2$SCAN XC | -0.5375 | 1.73 |

## V. MOLECULAR TEST SET DETAILED RESULTS

Here we provide the molecule-by-molecule tabulation for the G3/99, T96R, and T82-F test sets for *rreg*TM compared with *sreg*TM and, r$^2$SCAN, and PBE.

TABLE IX: Standard enthalpies of formation ($\Delta H_f$) in kcal/mol for the G3X/99 molecular test set [6, 7] obtained with different approximate exchange-correlation functionals.

| Molecule | Exp. | XC | *rreg*TM *rreg*TM | *v1-sreg*TM *rreg*TM | *v2-sreg*TM *rreg*TM | *v3-sreg*TM *rreg*TM | *rreg*TM *PBE* | *v2-sreg*TM *PBE* | r$^2$SCAN r$^2$SCAN | *PBE* *PBE* |
|---|---|---|---|---|---|---|---|---|---|---|
| LiH | 33.30 | | 35.971 | 35.928 | 35.926 | 35.945 | 38.861 | 38.815 | 36.369 | 38.353 |
| $^2$BeH | 81.70 | | 76.928 | 77.007 | 77.000 | 77.005 | 74.458 | 74.531 | 72.401 | 77.032 |
| $^2$CH | 142.50 | | 141.528 | 141.970 | 141.954 | 141.938 | 140.283 | 140.695 | 145.246 | 141.870 |
| $CH_2$ ($^3B_1$) | 93.60 | | 91.154 | 90.563 | 90.538 | 90.318 | 92.444 | 91.891 | 87.380 | 89.512 |
| $CH_2$ ($^1A_1$) | 102.60 | | 106.085 | 107.298 | 107.274 | 107.033 | 104.267 | 105.401 | 109.080 | 104.969 |
| $^3CH_3$ | 35.00 | | 33.582 | 34.330 | 34.291 | 33.897 | 34.199 | 34.936 | 31.093 | 32.400 |
| $CH_4$ | -17.80 | | -16.031 | -14.334 | -14.357 | -14.887 | -15.474 | -13.697 | -16.985 | -18.051 |
| $^3$NH | 85.80 | | 77.885 | 78.929 | 78.907 | 78.911 | 78.469 | 79.532 | 84.819 | 80.598 |
| $NH_2$ ($^2B_1$) | 44.50 | | 36.237 | 38.863 | 38.827 | 38.547 | 37.917 | 40.560 | 43.940 | 38.882 |
| $NH_3$ | -10.90 | | -13.125 | -10.482 | -10.516 | -11.007 | -9.982 | -7.192 | -6.591 | -14.099 |
| $^2$OH | 9.00 | | 7.318 | 8.397 | 8.412 | 8.140 | 9.887 | 11.021 | 7.906 | 6.631 |
| $H_2O$ | -57.80 | | -51.789 | -51.939 | -51.885 | -52.383 | -46.419 | -46.389 | -54.083 | -58.172 |
| HF | -65.20 | | -57.560 | -59.793 | -59.707 | -59.918 | -53.818 | -55.930 | -61.578 | -65.067 |
| $SiH_2$ ($^1A_1$) | 65.20 | | 67.435 | 67.561 | 67.616 | 67.642 | 64.694 | 64.883 | 67.659 | 68.485 |
| $SiH_2$ ($^3B_1$) | 86.20 | | 82.278 | 82.201 | 82.261 | 82.192 | 80.983 | 81.012 | 78.683 | 84.892 |
| $^2SiH_3$ | 47.90 | | 46.509 | 46.709 | 46.795 | 46.771 | 43.165 | 43.465 | 43.307 | 50.421 |
| $SiH_4$ | 8.20 | | 10.934 | 11.302 | 11.422 | 11.436 | 5.678 | 6.161 | 8.051 | 16.150 |
| $^2PH_2$ | 33.10 | | 27.532 | 29.353 | 29.389 | 29.341 | 26.007 | 27.951 | 30.299 | 31.274 |
| $PH_3$ | 1.30 | | -0.138 | 2.117 | 2.198 | 2.092 | -2.698 | -0.249 | 2.916 | 3.543 |
| $H_2S$ | -4.90 | | -4.547 | -3.322 | -3.314 | -3.590 | -3.730 | -2.315 | -4.802 | -4.615 |
| HCl | -22.00 | | -19.767 | -20.186 | -20.189 | -20.376 | -18.195 | -18.496 | -21.697 | -21.934 |
| $Li_2$ | 51.60 | | 55.210 | 55.257 | 55.253 | 55.260 | 57.583 | 57.626 | 57.947 | 56.191 |
| LiF | -80.10 | | -71.221 | -74.047 | -73.943 | -73.997 | -68.016 | -70.754 | -75.223 | -79.231 |
| HC≡CH | 54.60 | | 56.056 | 54.952 | 54.842 | 54.378 | 57.908 | 56.714 | 57.291 | 45.137 |
| $H_2C{=}CH_2$ | 12.50 | | 12.473 | 14.163 | 14.063 | 13.355 | 12.510 | 14.350 | 13.271 | 4.228 |
| $H_3C{-}CH_3$ | -20.10 | | -18.685 | -15.776 | -15.872 | -16.808 | -18.341 | -15.200 | -19.899 | -25.214 |
| CN | 105.20 | | 97.117 | 96.064 | 95.991 | 95.935 | 99.331 | 98.190 | 108.285 | 89.042 |
| HCN | 30.90 | | 26.818 | 26.609 | 26.513 | 26.299 | 27.352 | 27.082 | 36.347 | 18.183 |
| CO | -26.40 | | -24.030 | -26.272 | -26.197 | -26.385 | -22.623 | -24.768 | -22.494 | -36.038 |
| $^2$HCO | 10.00 | | 4.887 | 3.481 | 3.544 | 3.252 | 7.436 | 6.123 | 6.377 | -6.433 |
| $H_2CO$ | -26.10 | | -25.914 | -26.645 | -26.585 | -26.994 | -25.283 | -25.910 | -25.490 | -38.135 |
| $CH_3OH$ | -48.00 | | -44.995 | -44.358 | -44.273 | -44.970 | -42.189 | -41.343 | -46.549 | -55.038 |
| $N_2$ | 0.00 | | -9.460 | -8.139 | -8.310 | -8.285 | -10.606 | -9.381 | 8.712 | -14.907 |
| $H_2NNH_2$ | 23.30 | | 17.194 | 21.697 | 21.633 | 21.013 | 20.193 | 24.896 | 32.413 | 12.788 |
| NO | 21.80 | | 10.387 | 11.001 | 10.969 | 10.953 | 11.044 | 11.676 | 22.182 | 2.200 |
| $^3O_2$ | 0.00 | | -11.362 | -12.034 | -11.978 | -12.129 | -8.723 | -9.316 | -9.495 | -23.578 |
| $H_2O_2$ | -32.40 | | -34.134 | -33.284 | -33.107 | -33.590 | -29.115 | -27.951 | -31.281 | -45.264 |
| $F_2$ | 0.00 | | -4.972 | -6.102 | -5.876 | -5.741 | -5.078 | -5.948 | -0.542 | -14.480 |
| $CO_2$ | -94.00 | | -96.615 | -101.785 | -101.750 | -102.179 | -92.242 | -97.391 | -99.730 | -121.233 |
| $Na_2$ | 34.00 | | 33.438 | 33.542 | 33.547 | 33.550 | 36.049 | 36.162 | 37.360 | 33.232 |
| $Si_2$ | 139.90 | | 139.133 | 137.328 | 137.319 | 137.345 | 141.270 | 139.427 | 140.050 | 133.292 |
| $P_2$ | 34.30 | | 31.796 | 31.593 | 31.588 | 31.739 | 31.492 | 31.340 | 38.906 | 29.927 |
| $^3S_2$ | 30.70 | | 22.098 | 21.222 | 21.211 | 21.184 | 24.059 | 23.224 | 21.557 | 17.177 |

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| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| $Cl_2$ | 0.00 | -0.869 | -2.089 | -1.991 | -1.912 | -0.865 | -1.919 | -1.173 | -7.570 |
| NaCl | -43.60 | -38.153 | -40.030 | -39.969 | -40.077 | -36.560 | -38.386 | -42.209 | -39.225 |
| SiO | -24.60 | -19.203 | -21.605 | -21.404 | -21.479 | -17.387 | -19.597 | -19.627 | -27.933 |
| CS | 66.90 | 67.008 | 65.138 | 65.091 | 64.991 | 68.130 | 66.335 | 69.398 | 58.405 |
| SO | 1.20 | -5.856 | -6.848 | -6.696 | -6.800 | -3.628 | -4.428 | -5.788 | -14.255 |
| ClO | 24.30 | 15.738 | 15.584 | 15.690 | 15.703 | 16.652 | 16.666 | 18.816 | 7.982 |
| ClF | -13.30 | -14.689 | -16.160 | -15.961 | -15.846 | -14.769 | -15.989 | -13.513 | -23.623 |
| $Si_2H_6$ | 19.10 | 20.408 | 21.827 | 22.010 | 21.856 | 11.356 | 13.019 | 16.115 | 28.424 |
| $CH_3Cl$ | -19.60 | -18.575 | -18.502 | -18.498 | -18.921 | -18.492 | -18.311 | -20.538 | -25.231 |
| $H_3C-SH$ | -5.50 | -5.523 | -3.735 | -3.774 | -4.374 | -5.148 | -3.086 | -6.357 | -10.501 |
| HOCl | -18.40 | -19.367 | -19.592 | -19.445 | -19.646 | -16.849 | -16.816 | -18.260 | -28.359 |
| $SO_2$ | -71.00 | -71.260 | -74.905 | -74.613 | -74.828 | -68.025 | -71.332 | -72.660 | -91.183 |
| $BF_3$ | -271.40 | -258.398 | -267.343 | -266.884 | -267.240 | -253.001 | -261.526 | -273.732 | -282.638 |
| $BCl_3$ | -96.30 | -96.457 | -101.249 | -101.186 | -101.635 | -93.220 | -97.696 | -106.297 | -110.171 |
| $AlF_3$ | -289.00 | -269.775 | -278.657 | -278.277 | -278.523 | -265.504 | -274.062 | -286.282 | -287.468 |
| $AlCl_3$ | -139.70 | -135.310 | -141.287 | -141.054 | -141.410 | -132.864 | -138.614 | -147.936 | -140.648 |
| $CF_4$ | -223.10 | -217.478 | -228.411 | -227.853 | -227.998 | -212.131 | -222.543 | -229.516 | -250.932 |
| $CCl_4$ | -22.90 | -25.064 | -30.435 | -30.434 | -30.539 | -22.652 | -27.643 | -29.324 | -44.635 |
| OCS | -33.10 | -40.292 | -44.547 | -44.541 | -44.882 | -36.797 | -40.958 | -42.142 | -59.555 |
| $CS_2$ | 28.00 | 18.381 | 14.678 | 14.598 | 14.337 | 21.373 | 17.758 | 16.922 | 3.687 |
| $F_2CO$ | -145.00 | -144.300 | -152.159 | -151.854 | -152.134 | -139.523 | -147.085 | -151.353 | -174.364 |
| $SiF_4$ | -386.00 | -361.077 | -373.161 | -372.539 | -372.791 | -356.152 | -367.703 | -381.350 | -383.670 |
| $SiCl_4$ | -158.40 | -152.616 | -160.212 | -159.900 | -160.226 | -150.085 | -157.307 | -165.540 | -162.572 |
| NNO | 19.70 | -1.347 | -2.910 | -3.102 | -3.161 | 0.400 | -1.311 | 14.882 | -20.819 |
| ClNO | 12.60 | -5.187 | -6.938 | -6.901 | -6.898 | -3.620 | -5.256 | 5.366 | -21.066 |
| $NF_3$ | -31.60 | -49.226 | -53.398 | -53.044 | -52.785 | -47.882 | -51.654 | -40.578 | -71.956 |
| $PF_3$ | -229.10 | -220.179 | -227.436 | -226.830 | -226.748 | -218.215 | -224.894 | -226.170 | -239.427 |
| $O_3$ | 33.90 | 19.396 | 18.388 | 18.573 | 18.537 | 21.805 | 21.096 | 29.247 | -3.619 |
| $F_2O$ | 5.90 | -8.284 | -9.714 | -9.364 | -9.209 | -7.902 | -8.912 | -1.016 | -24.698 |
| $ClF_3$ | -38.00 | -51.706 | -57.418 | -56.919 | -56.625 | -48.937 | -54.115 | -52.045 | -76.974 |
| $F_2C=CF_2$ | -161.30 | -162.865 | -173.293 | -172.793 | -173.119 | -157.518 | -167.401 | -170.535 | -204.597 |
| $Cl_2C=CCl_2$ | -5.50 | -10.301 | -16.504 | -16.672 | -17.032 | -7.064 | -12.968 | -14.830 | -38.126 |
| $F_3C-CN$ | -118.40 | -124.320 | -132.204 | -131.919 | -132.286 | -120.187 | -127.682 | -121.756 | -160.508 |
| $HC\equiv C-CH_3$ | 44.40 | 44.298 | 44.127 | 43.923 | 42.999 | 46.741 | 46.624 | 44.560 | 28.038 |
| $H_2C=C=CH_2$ | 45.40 | 40.595 | 41.211 | 40.997 | 40.054 | 42.603 | 43.372 | 41.757 | 24.612 |
| $C_3H_4$ (cyclopropene) | 67.80 | 63.614 | 63.715 | 63.498 | 62.712 | 65.251 | 65.508 | 65.517 | 47.295 |
| $H_2C=CH-CH_3$ | 4.80 | 3.765 | 6.666 | 6.483 | 5.334 | 4.236 | 7.432 | 4.184 | -8.811 |
| $C_3H_6$ (cyclopropane) | 12.80 | 10.652 | 12.384 | 12.159 | 11.141 | 11.652 | 13.638 | 10.333 | -2.957 |
| $CH_3-CH_2-CH_3$ | -25.10 | -24.064 | -19.883 | -20.048 | -21.389 | -23.756 | -19.191 | -25.256 | -34.289 |
| $C_4H_6$ (Z-1,3-butadiene) | 26.40 | 22.152 | 25.167 | 24.901 | 23.547 | 22.389 | 25.744 | 24.253 | 3.800 |
| $C_4H_6$ (2-butyne) | 34.80 | 34.304 | 34.998 | 34.699 | 33.334 | 37.176 | 38.067 | 33.601 | 12.610 |
| $C_4H_6$ (methylenecyclopropane) | 47.90 | 40.161 | 41.648 | 41.325 | 40.080 | 41.972 | 43.782 | 41.192 | 19.512 |
| $C_4H_6$ (bicyclo[1.1.0]butane) | 51.90 | 46.936 | 47.503 | 47.171 | 46.081 | 48.920 | 49.685 | 48.326 | 26.702 |
| $C_4H_6$ (cyclobutene) | 38.20 | 33.235 | 36.481 | 36.265 | 34.936 | 33.373 | 37.117 | 36.791 | 14.490 |
| $C_4H_8$ (cyclobutane) | 6.60 | 3.500 | 8.128 | 7.924 | 6.395 | 3.135 | 8.349 | 5.204 | -12.675 |
| $C_4H_8$ (isobutene) | -4.10 | -5.710 | -1.527 | -1.784 | -3.363 | -4.892 | -0.281 | -5.292 | -21.712 |
| $C_4H_{10}$ (trans butane) | -30.10 | -29.393 | -23.955 | -24.188 | -25.935 | -29.122 | -23.148 | -30.572 | -43.284 |
| $C_4H_{10}$ (isobutane) | -32.20 | -31.423 | -25.913 | -26.139 | -27.880 | -31.056 | -25.019 | -32.187 | -44.374 |
| $C_5H_8$ (spiropentane) | 44.30 | 37.107 | 39.006 | 38.575 | 37.049 | 39.162 | 41.479 | 37.527 | 11.935 |
| $C_6H_6$ (benzene) | 19.90 | 7.780 | 11.253 | 10.751 | 8.821 | 8.284 | 12.330 | 10.403 | -22.848 |
| $CH_2F_2$ | -107.70 | -104.204 | -108.414 | -108.092 | -108.337 | -103.184 | -107.109 | -109.028 | -122.140 |
| $CHF_3$ | -166.30 | -162.018 | -169.598 | -169.145 | -169.322 | -159.077 | -166.249 | -170.262 | -187.903 |

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| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| $CH_2Cl_2$ | -22.60 | -22.346 | -24.127 | -24.119 | -24.440 | -21.910 | -23.521 | -25.527 | -33.914 |
| $CHCl_3$ | -24.50 | -25.176 | -28.817 | -28.816 | -29.034 | -23.854 | -27.233 | -29.246 | -41.183 |
| $CH_3NH_2$ | -5.20 | -0.375 | 3.134 | 3.078 | 2.289 | 0.917 | 4.643 | 5.683 | -5.273 |
| $CH_3CN$ | 18.00 | 11.856 | 12.545 | 12.359 | 11.678 | 12.990 | 13.763 | 20.217 | -2.068 |
| $CH_3NO_2$ (nitromethane) | -17.90 | -35.174 | -35.093 | -35.135 | -35.724 | -33.259 | -32.960 | -25.879 | -59.555 |
| $CH_3ONO$ (methyl nitrite) | -16.10 | -32.835 | -32.874 | -32.778 | -33.238 | -31.509 | -31.293 | -21.287 | -54.847 |
| $CH_3SiH_3$ | -7.00 | -3.502 | -1.984 | -1.883 | -2.416 | -6.960 | -5.122 | -7.007 | -2.305 |
| $HCO_2H$ | -90.40 | -90.503 | -93.200 | -93.062 | -93.710 | -85.567 | -88.011 | -93.046 | -111.954 |
| $HCO_2CH_3$ | -85.50 | -88.070 | -89.998 | -89.807 | -90.647 | -85.711 | -87.341 | -89.540 | -111.885 |
| $CH_3CONH_2$ | -57.00 | -64.185 | -62.589 | -62.664 | -63.867 | -59.880 | -57.904 | -58.876 | -84.231 |
| $C_2H_5N$ (aziridine) | 30.20 | 21.742 | 24.060 | 23.947 | 23.195 | 22.658 | 25.197 | 30.296 | 10.031 |
| NCCN (cyanogen) | 74.10 | 57.991 | 56.920 | 56.628 | 56.248 | 59.282 | 58.096 | 77.596 | 37.081 |
| $NH(CH_3)_2$ | -4.30 | -8.323 | -4.227 | -4.316 | -5.366 | -7.916 | -3.513 | -1.721 | -17.806 |
| $CH_3CH_2NH_2$ | -11.30 | -15.894 | -11.270 | -11.398 | -12.582 | -14.069 | -9.052 | -9.440 | -25.203 |
| $H_2C{=}C{=}O$ (ketene) | -11.60 | -16.890 | -19.237 | -19.314 | -20.013 | -13.082 | -15.299 | -17.674 | -37.267 |
| $C_2H_4O$ (oxirane) | -12.60 | -16.956 | -16.660 | -16.563 | -17.208 | -16.229 | -15.658 | -15.115 | -32.026 |
| $CH_3CHO$ | -39.50 | -40.873 | -40.396 | -40.420 | -41.303 | -39.372 | -38.611 | -41.209 | -57.475 |
| $O{=}CH{-}CH{=}O$ | -50.80 | -54.597 | -56.230 | -56.157 | -56.944 | -52.833 | -54.157 | -52.935 | -80.457 |
| $CH_3CH_2OH$ | -56.10 | -53.946 | -51.946 | -51.927 | -53.052 | -50.992 | -48.616 | -55.501 | -67.563 |
| $(CH_3)_2O$ | -44.00 | -43.489 | -42.119 | -41.997 | -42.887 | -43.151 | -41.531 | -44.134 | -56.457 |
| $C_2H_4S$ (thiooxirane) | 19.60 | 14.486 | 15.219 | 15.142 | 14.512 | 14.950 | 15.899 | 15.131 | 2.869 |
| $(CH_3)_2S{=}O$ | -36.20 | -38.239 | -36.977 | -36.976 | -38.054 | -36.313 | -34.504 | -40.593 | -55.337 |
| $CH_3CH_2SH$ | -11.10 | -11.299 | -8.284 | -8.389 | -9.389 | -10.921 | -7.478 | -12.118 | -19.965 |
| $(CH_3)_2S$ | -8.90 | -9.578 | -7.235 | -7.328 | -8.260 | -9.362 | -6.644 | -10.926 | -19.041 |
| $H_2C{=}CHF$ | -34.00 | -34.775 | -36.014 | -35.950 | -36.561 | -33.487 | -34.467 | -35.880 | -51.223 |
| $CH_3CH_2Cl$ | -26.60 | -26.379 | -25.055 | -25.114 | -25.953 | -26.168 | -24.574 | -28.392 | -36.728 |
| $H_2C{=}CHCl$ | 5.20 | 3.547 | 3.291 | 3.183 | 2.545 | 4.367 | 4.300 | 2.760 | -9.818 |
| $H_2C{=}CHCN$ | 43.20 | 35.738 | 36.547 | 36.280 | 35.411 | 36.501 | 37.435 | 46.042 | 15.936 |
| $(CH_3)_2C{=}O$ | -51.70 | -53.966 | -52.199 | -52.295 | -53.634 | -51.799 | -49.578 | -54.629 | -73.961 |
| $CH_3CO_2H$ | -103.40 | -104.124 | -105.368 | -105.301 | -106.424 | -98.510 | -99.338 | -106.948 | -128.749 |
| $CH_3CFO$ | -105.70 | -106.396 | -109.301 | -109.179 | -109.984 | -103.017 | -105.555 | -109.997 | -131.162 |
| $CH_3COCl$ | -57.70 | -61.889 | -63.982 | -63.993 | -64.800 | -58.797 | -60.610 | -64.631 | -83.546 |
| $CH_3CH_2CH_2Cl$ | -31.50 | -31.636 | -29.087 | -29.214 | -30.455 | -31.474 | -28.506 | -33.686 | -45.698 |
| $(CH_3)_2CHOH$ | -65.20 | -63.969 | -60.593 | -60.636 | -62.180 | -60.734 | -56.820 | -65.178 | -80.323 |
| $CH_3{-}O{-}CH_2CH_3$ | -51.70 | -52.283 | -49.553 | -49.498 | -50.818 | -51.787 | -48.641 | -52.970 | -68.837 |
| $(CH_3)_3N$ | -6.60 | -11.277 | -6.450 | -6.558 | -7.875 | -12.139 | -6.923 | -4.148 | -23.659 |
| $C_4H_4O$ (furan) | -8.30 | -17.416 | -17.826 | -17.894 | -19.124 | -15.088 | -15.022 | -15.438 | -46.264 |
| $C_4H_4S$ (thiophene) | 27.50 | 18.128 | 18.525 | 18.184 | 16.937 | 19.832 | 20.730 | 18.924 | -6.991 |
| $C_4H_5N$ (pyrrole) | 25.90 | 11.965 | 14.081 | 13.806 | 12.408 | 14.275 | 16.834 | 20.536 | -13.692 |
| $C_5H_5N$ (pyridine) | 33.60 | 15.585 | 18.805 | 18.374 | 16.784 | 15.252 | 19.005 | 25.893 | -14.365 |
| $H_2$ | 0.00 | 1.322 | 1.322 | 1.322 | 1.322 | 3.877 | 3.877 | 2.029 | 4.886 |
| $^2SH$ | 34.20 | 32.088 | 33.096 | 33.094 | 32.954 | 32.629 | 33.713 | 32.445 | 33.105 |
| $^2C{\equiv}CH$ | 135.80 | 134.024 | 132.370 | 132.258 | 131.913 | 136.932 | 135.206 | 134.490 | 123.889 |
| $HC{=}CH_2$ ($^2A'$) | 71.00 | 65.965 | 66.756 | 66.638 | 66.034 | 67.630 | 68.485 | 66.139 | 58.415 |
| $CH_3C{=}O$ ($^2A'$) | -2.40 | -8.747 | -8.994 | -8.999 | -9.746 | -5.786 | -5.808 | -8.016 | -24.710 |
| $CH_2{-}OH$ ($^2A$) | -4.00 | -5.907 | -6.037 | -5.957 | -6.549 | -2.063 | -2.017 | -7.899 | -15.885 |
| $CH_3O$ ($^2A'$) | 5.20 | -1.823 | -0.487 | -0.441 | -0.959 | -0.553 | 0.953 | -1.003 | -8.513 |
| $CH_3CH_2O$ ($^2A''$) | -2.90 | -11.455 | -8.857 | -8.881 | -9.834 | -9.810 | -6.862 | -10.758 | -22.343 |
| $CH_3S$ ($^2A'$) | 29.80 | 25.697 | 27.136 | 27.084 | 26.605 | 26.252 | 27.874 | 25.434 | 21.234 |
| $CH_2CH_3$ ($^2A'$) | 28.60 | 26.062 | 28.013 | 27.898 | 27.057 | 27.160 | 29.235 | 23.478 | 19.913 |
| $(CH_3)_2CH$ ($^2A'$) | 21.10 | 17.254 | 20.434 | 20.243 | 18.963 | 18.827 | 22.260 | 14.611 | 6.724 |
| $^2C(CH_3)_3$ | 12.00 | 7.741 | 12.181 | 11.922 | 10.214 | 9.683 | 14.501 | 5.238 | -6.483 |

(continued)

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| $NO_2$ ($^2A_1$) | 8.10 | -13.683 | -15.203 | -15.256 | -15.378 | -10.710 | -12.234 | -3.219 | -34.634 |
| $CH_3CH{=}C{=}CH_2$ | 38.80 | 33.842 | 35.560 | 35.268 | 33.913 | 35.948 | 37.954 | 34.599 | 13.314 |
| $C_5H_8$ (isoprene) | 18.00 | 13.269 | 17.580 | 17.244 | 15.460 | 13.787 | 18.578 | 15.537 | -8.185 |
| $C_5H_{10}$ (cyclopentane twist) | -18.50 | -20.124 | -14.267 | -14.579 | -16.576 | -20.360 | -13.738 | -20.086 | -40.154 |
| $C_5H_{12}$ (n-pentane) | -35.00 | -34.655 | -27.959 | -28.262 | -30.413 | -34.432 | -27.050 | -35.811 | -52.206 |
| $C(CH_3)_4$ (neopentane) | -40.10 | -39.945 | -33.063 | -33.340 | -35.469 | -39.519 | -31.976 | -39.783 | -54.531 |
| $C_6H_8$ (1,3-cyclohexadiene) | 25.40 | 19.087 | 23.832 | 23.377 | 21.287 | 19.648 | 25.105 | 21.575 | -9.671 |
| $C_6H_8$ (1,4-cyclohexadiene) | 25.00 | 19.657 | 24.359 | 23.891 | 21.782 | 20.442 | 25.863 | 21.779 | -9.517 |
| $C_6H_{12}$ (cyclohexane chair) | -29.40 | -30.939 | -23.522 | -23.923 | -26.350 | -31.172 | -22.844 | -30.893 | -53.494 |
| $C_6H_{14}$ (n-hexane) | -39.90 | -39.936 | -31.983 | -32.355 | -34.910 | -39.757 | -30.966 | -41.090 | -61.144 |
| $C_6H_{14}$ (3-methylpentane) | -41.10 | -40.484 | -32.493 | -32.852 | -35.399 | -40.342 | -31.512 | -41.004 | -60.442 |
| $C_6H_5{-}CH_3$ (toluene) | 12.00 | -0.311 | 4.379 | 3.800 | 1.436 | 0.630 | 6.023 | 2.192 | -34.726 |
| $C_7H_{16}$ (n-heptane) | -44.80 | -45.208 | -35.999 | -36.439 | -39.399 | -45.074 | -34.875 | -46.317 | -70.074 |
| $C_8H_8$ (cyclooctatetraene) | 70.70 | 59.547 | 64.454 | 63.800 | 61.253 | 60.564 | 66.287 | 65.076 | 18.532 |
| $C_8H_{18}$ (n-octane) | -49.80 | -50.491 | -40.024 | -40.534 | -43.898 | -50.401 | -38.794 | -51.578 | -79.015 |
| $C_{10}H_8$ (naphtalene) | 35.90 | 12.133 | 17.592 | 16.698 | 13.551 | 13.144 | 19.578 | 17.424 | -40.015 |
| $C_{10}H_8$ (azulene) | 69.10 | 43.747 | 49.017 | 48.147 | 45.047 | 45.091 | 51.337 | 50.165 | -9.667 |
| $CH_3CO_2CH_3$ (Z-methylacetate) | -98.40 | -101.175 | -101.667 | -101.548 | -102.858 | -98.182 | -98.209 | -102.893 | -128.162 |
| $(CH_3)_3COH$ (t-butanol) | -74.70 | -74.214 | -69.403 | -69.498 | -71.452 | -70.725 | -65.227 | -74.627 | -92.259 |
| $C_6H_5NH_2$ (aniline) | 20.80 | 1.796 | 6.592 | 6.037 | 3.807 | 4.965 | 10.447 | 11.151 | -32.284 |
| $C_6H_5OH$ (phenol) | -22.30 | -34.941 | -32.859 | -33.266 | -35.426 | -30.508 | -27.717 | -33.497 | -73.497 |
| $C_4H_6O$ (divinyl ether) | -3.30 | -8.750 | -7.904 | -7.958 | -9.333 | -6.590 | -5.319 | -7.406 | -35.231 |
| $C_4H_8O$ (tetrahydrofuran) | -44.00 | -46.020 | -42.825 | -42.859 | -44.443 | -45.871 | -42.019 | -45.741 | -68.725 |
| $C_5H_8O$ (cyclopentanone) | -45.90 | -51.375 | -48.082 | -48.342 | -50.348 | -49.466 | -45.342 | -51.377 | -81.653 |
| $C_6H_4O_2$ (benzoquinone) | -29.40 | -43.777 | -42.927 | -43.227 | -45.260 | -41.541 | -39.911 | -38.774 | -90.551 |
| $C_6H_4N_2$ (pyrimidine) | 46.80 | 21.576 | 24.416 | 24.048 | 22.800 | 20.482 | 23.810 | 39.251 | -7.724 |
| $(CH_3)_2SO_2$ | -89.20 | -89.810 | -90.004 | -89.919 | -91.247 | -85.931 | -85.520 | -95.574 | -113.367 |
| $C_6H_5Cl$ (chlorobenzene) | 12.50 | -1.026 | 0.454 | -0.051 | -1.900 | 0.291 | 2.376 | 0.253 | -36.164 |
| $NC(CH_2)_2CN$ (succinonitrile) | 50.10 | 36.718 | 37.708 | 37.301 | 36.084 | 38.262 | 39.480 | 54.670 | 7.507 |
| $C_4H_4N_2$ (pyrazine) | 46.90 | 25.091 | 28.171 | 27.817 | 26.567 | 23.921 | 27.497 | 43.407 | -4.086 |
| $C_4H_4O$ (3-butyn-2-one) | 15.60 | 13.813 | 12.712 | 12.512 | 11.223 | 17.502 | 16.643 | 15.244 | -15.729 |
| $C_4H_6O$ (E-crotonaldehyde) | -24.00 | -30.522 | -28.702 | -28.889 | -30.407 | -29.057 | -26.767 | -29.433 | -57.070 |
| $C_4H_6O_3$ (acetic anhydride) | -136.80 | -143.885 | -146.238 | -146.158 | -147.889 | -137.906 | -139.608 | -146.708 | -185.596 |
| $C_4H_6S$ (2,5-dihydrothiophene) | 20.80 | 14.933 | 17.559 | 17.289 | 15.868 | 15.207 | 18.484 | 15.945 | -7.106 |
| $(CH_3)_2CHCN$ | 5.60 | 0.675 | 3.919 | 3.613 | 2.144 | 1.574 | 5.187 | 9.229 | -20.146 |
| $C_4H_8O$ (methyl ethyl ketone) | -57.10 | -59.733 | -56.712 | -56.875 | -58.619 | -57.576 | -53.944 | -60.325 | -83.160 |
| $(CH_3)_2CHCHO$ | -51.60 | -52.191 | -49.283 | -49.434 | -51.098 | -50.804 | -47.331 | -52.368 | -75.639 |
| $C_4H_8O_2$ (1,4-dioxane) | -75.50 | -79.758 | -77.661 | -77.480 | -79.077 | -79.218 | -76.407 | -78.669 | -107.583 |
| $C_4H_8S$ (tetrahydrothiophene) | -8.20 | -10.845 | -6.875 | -7.109 | -8.689 | -11.100 | -6.394 | -10.968 | -29.721 |
| $(CH_3)_3CCl$ | -43.50 | -45.017 | -40.904 | -41.065 | -42.717 | -44.447 | -39.763 | -45.684 | -59.576 |
| $C_4H_9Cl$ (n-butyl chloride) | -37.00 | -36.835 | -33.033 | -33.228 | -34.871 | -36.740 | -32.370 | -38.869 | -54.560 |
| $C_4H_9N$ (tetrahydropyrrole) | -0.80 | -8.067 | -2.167 | -2.393 | -4.117 | -8.140 | -1.532 | -0.164 | -27.032 |
| $C_4H_9NO_2$ (2-nitrobutane) | -39.10 | -57.293 | -53.427 | -53.657 | -55.462 | -55.156 | -50.604 | -47.460 | -90.951 |
| $(CH_3CH_2)_2O$ | -60.30 | -60.959 | -56.874 | -56.886 | -58.634 | -60.320 | -55.651 | -61.704 | -81.093 |
| $CH_3CH(OCH_3)_2$ (dimethyl acetal) | -93.10 | -94.781 | -92.514 | -92.304 | -94.010 | -93.481 | -90.591 | -95.091 | -119.944 |
| $(CH_3)_3CSH$ | -26.20 | -28.123 | -22.438 | -22.649 | -24.433 | -27.482 | -21.083 | -27.472 | -41.107 |
| $C_4H_{10}S_2$ (diethyl disulfide) | -17.90 | -20.993 | -16.792 | -17.002 | -18.709 | -20.505 | -15.554 | -22.447 | -41.111 |
| $(CH_3)_3CNH_2$ | -28.90 | -34.252 | -26.808 | -27.045 | -29.039 | -32.125 | -24.000 | -26.378 | -47.647 |
| $(CH_3)_4Si$ | -55.70 | -49.712 | -44.601 | -44.539 | -46.710 | -47.136 | -41.109 | -54.175 | -58.530 |
| $C_5H_6S$ (2-methyl thiophene) | 20.00 | 10.233 | 11.809 | 11.390 | 9.717 | 12.277 | 14.483 | 10.745 | -18.880 |
| $C_5H_7N$ (N-methyl pyrrole) | 24.60 | 10.345 | 13.132 | 12.838 | 11.152 | 11.465 | 14.779 | 18.955 | -19.073 |
| $C_5H_{10}O$ (tetrahydropyran) | -53.40 | -56.001 | -51.304 | -51.416 | -53.428 | -55.810 | -50.295 | -55.557 | -81.279 |

(continued)

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| $(CH_3CH_2)_2C{=}O$ | -61.60 | -65.396 | -61.130 | -61.358 | -63.507 | -63.262 | -58.227 | -65.921 | -92.252 |
| $C_5H_{10}O_2$ (isopropyl acetate) | -115.10 | -119.100 | -116.863 | -116.873 | -119.037 | -115.704 | -112.678 | -120.534 | -152.246 |
| $C_5H_{10}S$ (tetrahydrothiopyran) | -15.20 | -18.290 | -12.763 | -13.089 | -15.104 | -18.488 | -12.055 | -18.399 | -40.167 |
| $C_5H_{11}N$ (piperidine) | -11.30 | -18.181 | -10.877 | -11.196 | -13.345 | -18.020 | -9.852 | -10.425 | -39.964 |
| $C_5H_{12}O$ (t-butyl methyl ether) | -67.80 | -69.190 | -63.659 | -63.713 | -65.858 | -68.289 | -62.025 | -68.525 | -89.665 |
| $C_6H_4F_2$ (1,3-difluorobenzene) | -73.90 | -87.740 | -90.078 | -90.254 | -92.018 | -84.300 | -85.869 | -88.648 | -133.695 |
| $C_6H_4F_2$ (1,4-difluorobenzene) | -73.30 | -86.982 | -89.302 | -89.478 | -91.237 | -83.608 | -85.164 | -87.757 | -132.983 |
| $C_6H_5F$ (fluorobenzene) | -27.40 | -40.311 | -39.750 | -40.088 | -41.933 | -38.346 | -37.115 | -39.430 | -78.603 |
| $C_6H_{14}O$ (diisopropyl ether) | -76.30 | -78.020 | -71.166 | -71.295 | -73.875 | -77.025 | -69.263 | -77.839 | -103.079 |
| $PF_5$ | -381.10 | -364.825 | -377.789 | -376.790 | -376.879 | -359.910 | -371.940 | -380.254 | -391.911 |
| $SF_6$ | -291.70 | -289.541 | -303.559 | -302.412 | -302.338 | -283.071 | -295.991 | -303.621 | -323.703 |
| $P_4$ | 14.10 | -4.250 | -4.575 | -4.554 | -4.063 | -4.603 | -4.811 | 9.944 | -6.429 |
| $SO_3$ | -94.60 | -97.506 | -103.477 | -103.157 | -103.549 | -91.963 | -97.609 | -102.558 | -125.370 |
| $SCl_2$ | -4.20 | -7.894 | -10.166 | -10.036 | -9.944 | -7.254 | -9.299 | -9.243 | -18.677 |
| $POCl_3$ | -133.80 | -134.339 | -140.596 | -140.310 | -140.495 | -131.249 | -137.130 | -140.862 | -151.623 |
| $PCl_5$ | -86.10 | -94.488 | -101.034 | -100.744 | -100.696 | -91.907 | -98.031 | -99.199 | -108.417 |
| $Cl_2O_2S$ | -84.80 | -89.446 | -96.189 | -95.918 | -96.150 | -84.102 | -90.533 | -96.999 | -116.410 |
| $PCl_3$ | -69.00 | -72.323 | -76.457 | -76.270 | -76.188 | -70.937 | -74.824 | -74.777 | -83.704 |
| $Cl_2S_2$ | -4.00 | -15.860 | -19.236 | -19.103 | -19.007 | -13.790 | -16.868 | -18.120 | -31.124 |
| $SiCl_2$ ($^1A_1$) | -40.30 | -37.993 | -42.201 | -42.012 | -42.066 | -36.377 | -40.401 | -42.734 | -46.440 |
| $CF_3Cl$ | -169.70 | -167.901 | -177.302 | -176.882 | -177.026 | -163.341 | -172.236 | -177.683 | -197.941 |
| $C_2F_6$ | -320.90 | -318.228 | -333.038 | -332.161 | -332.512 | -311.386 | -325.326 | -332.636 | -367.896 |
| $^2CF_3$ | -111.80 | -113.522 | -121.704 | -121.275 | -121.388 | -109.001 | -116.788 | -122.127 | -139.910 |
| $^2C_6H_5$ (phenyl radical) | 80.50 | 63.114 | 65.567 | 65.060 | 63.260 | 65.129 | 68.046 | 65.334 | 33.117 |
| ME | | -3.790 | -3.467 | -3.512 | -4.411 | -2.208 | -1.520 | -3.145 | -20.878 |
| MAD | | 5.612 | 5.885 | 5.895 | 6.128 | 5.452 | 5.354 | 4.488 | 21.385 |

TABLE X: Bond lengths in $\AA$ for the T96-R molecular test set [8, 9] from different approximate XC functionals.

| Molecule | Exp. | X C | *rreg*TM *rreg*TM | *v1-sreg*TM *rreg*TM | *v2-sreg*TM *rreg*TM | *v3-sreg*TM *rreg*TM | *rreg*TM *PBE* | *v2-sreg*TM *PBE* | r$^2$SCAN r$^2$SCAN | *PBE* *PBE* |
|---|---|---|---|---|---|---|---|---|---|---|
| $H_2$ | 0.741 | | 0.744 | 0.744 | 0.744 | 0.744 | 0.743 | 0.743 | 0.742 | 0.751 |
| $Li_2$ | 2.673 | | 2.731 | 2.736 | 2.736 | 2.736 | 2.738 | 2.744 | 2.762 | 2.738 |
| LiH | 1.595 | | 1.606 | 1.606 | 1.606 | 1.607 | 1.595 | 1.595 | 1.605 | 1.607 |
| LiF | 1.564 | | 1.579 | 1.579 | 1.579 | 1.579 | 1.571 | 1.571 | 1.574 | 1.576 |
| LiCl | 2.021 | | 2.029 | 2.029 | 2.029 | 2.029 | 2.018 | 2.018 | 2.029 | 2.021 |
| LiO | 1.688 | | 1.702 | 1.703 | 1.703 | 1.702 | 1.691 | 1.692 | 1.696 | 1.699 |
| $Be_2$ | 2.440 | | 2.486 | 2.487 | 2.487 | 2.486 | 2.439 | 2.428 | 2.489 | 2.441 |
| BeH | 1.343 | | 1.359 | 1.360 | 1.360 | 1.360 | 1.351 | 1.351 | 1.357 | 1.362 |
| BeF | 1.361 | | 1.381 | 1.381 | 1.381 | 1.380 | 1.378 | 1.378 | 1.374 | 1.382 |
| BeO | 1.331 | | 1.344 | 1.344 | 1.344 | 1.344 | 1.340 | 1.340 | 1.335 | 1.346 |
| BeS | 1.742 | | 1.754 | 1.754 | 1.754 | 1.754 | 1.748 | 1.749 | 1.749 | 1.759 |
| $B_2$ | 1.590 | | 1.622 | 1.621 | 1.621 | 1.620 | 1.618 | 1.617 | 1.618 | 1.619 |
| BH | 1.232 | | 1.245 | 1.245 | 1.245 | 1.245 | 1.237 | 1.237 | 1.242 | 1.252 |
| BF | 1.263 | | 1.274 | 1.273 | 1.273 | 1.273 | 1.272 | 1.272 | 1.267 | 1.276 |
| $BF_3$ | 1.313 | | 1.322 | 1.321 | 1.321 | 1.321 | 1.320 | 1.319 | 1.314 | 1.325 |
| BCl | 1.715 | | 1.725 | 1.729 | 1.728 | 1.728 | 1.719 | 1.722 | 1.724 | 1.732 |
| $BCl_3$ | 1.742 | | 1.743 | 1.744 | 1.744 | 1.744 | 1.741 | 1.742 | 1.742 | 1.748 |
| BN | 1.281 | | 1.329 | 1.331 | 1.331 | 1.331 | 1.324 | 1.326 | 1.321 | 1.333 |
| BO | 1.204 | | 1.213 | 1.213 | 1.213 | 1.213 | 1.210 | 1.210 | 1.206 | 1.215 |
| BS | 1.609 | | 1.617 | 1.618 | 1.618 | 1.617 | 1.613 | 1.614 | 1.612 | 1.621 |
| $C_2$ | 1.242 | | 1.254 | 1.399 | 1.399 | 1.254 | 1.252 | 1.253 | 1.249 | 1.404 |
| CH | 1.120 | | 1.135 | 1.136 | 1.136 | 1.136 | 1.126 | 1.127 | 1.126 | 1.137 |
| $CH_4$ | 1.087 | | 1.092 | 1.093 | 1.093 | 1.092 | 1.089 | 1.090 | 1.088 | 1.096 |
| CF | 1.272 | | 1.288 | 1.287 | 1.287 | 1.286 | 1.286 | 1.285 | 1.278 | 1.287 |
| $CF_4$ | 1.323 | | 1.334 | 1.332 | 1.332 | 1.332 | 1.333 | 1.331 | 1.325 | 1.337 |
| CCl | 1.645 | | 1.663 | 1.663 | 1.663 | 1.662 | 1.661 | 1.661 | 1.654 | 1.660 |
| $CCl_4$ | 1.767 | | 1.777 | 1.778 | 1.778 | 1.778 | 1.773 | 1.775 | 1.774 | 1.782 |
| CN | 1.172 | | 1.172 | 1.173 | 1.173 | 1.173 | 1.170 | 1.171 | 1.165 | 1.174 |
| CO | 1.128 | | 1.133 | 1.134 | 1.134 | 1.134 | 1.132 | 1.133 | 1.127 | 1.136 |
| $CO^+$ | 1.115 | | 1.120 | 1.120 | 1.120 | 1.120 | 1.117 | 1.118 | 1.112 | 1.122 |
| $CO_2$ | 1.160 | | 1.169 | 1.169 | 1.169 | 1.169 | 1.168 | 1.168 | 1.162 | 1.171 |
| CP | 1.562 | | 1.562 | 1.562 | 1.562 | 1.562 | 1.558 | 1.559 | 1.555 | 1.567 |
| CS | 1.535 | | 1.541 | 1.543 | 1.543 | 1.542 | 1.538 | 1.540 | 1.536 | 1.546 |
| $CS_2$ | 1.553 | | 1.559 | 1.559 | 1.559 | 1.558 | 1.557 | 1.557 | 1.553 | 1.562 |
| $N_2$ | 1.098 | | 1.099 | 1.101 | 1.101 | 1.100 | 1.098 | 1.099 | 1.093 | 1.103 |
| $N_2^+$ | 1.116 | | 1.113 | 1.114 | 1.113 | 1.113 | 1.111 | 1.112 | 1.106 | 1.114 |
| NH | 1.036 | | 1.049 | 1.049 | 1.049 | 1.049 | 1.043 | 1.043 | 1.041 | 1.051 |
| $NH^+$ | 1.070 | | 1.087 | 1.088 | 1.088 | 1.088 | 1.078 | 1.080 | 1.078 | 1.091 |
| NF | 1.317 | | 1.332 | 1.329 | 1.329 | 1.328 | 1.331 | 1.328 | 1.319 | 1.327 |
| NCl | 1.611 | | 1.626 | 1.624 | 1.623 | 1.622 | 1.625 | 1.622 | 1.616 | 1.618 |
| NO | 1.151 | | 1.157 | 1.157 | 1.157 | 1.156 | 1.155 | 1.155 | 1.148 | 1.158 |
| $NO^+$ | 1.063 | | 1.066 | 1.067 | 1.067 | 1.067 | 1.064 | 1.065 | 1.059 | 1.070 |
| NS | 1.494 | | 1.504 | 1.504 | 1.504 | 1.503 | 1.502 | 1.501 | 1.494 | 1.506 |
| $O_2$ | 1.208 | | 1.220 | 1.219 | 1.218 | 1.218 | 1.219 | 1.218 | 1.207 | 1.219 |
| $O_2^+$ | 1.116 | | 1.121 | 1.120 | 1.120 | 1.120 | 1.119 | 1.119 | 1.109 | 1.122 |
| OH | 0.970 | | 0.981 | 0.982 | 0.982 | 0.981 | 0.978 | 0.979 | 0.973 | 0.983 |
| $OH^+$ | 1.029 | | 1.044 | 1.044 | 1.044 | 1.044 | 1.037 | 1.037 | 1.035 | 1.048 |
| OF | 1.358 | | 1.367 | 1.364 | 1.364 | 1.364 | 1.368 | 1.365 | 1.350 | 1.360 |
| $F_2$ | 1.412 | | 1.417 | 1.415 | 1.415 | 1.414 | 1.417 | 1.415 | 1.399 | 1.413 |

(continued)

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| $F_2^+$ | 1.322 | 1.317 | 1.315 | 1.315 | 1.315 | 1.317 | 1.315 | 1.298 | 1.316 |
| HF | 0.917 | 0.929 | 0.929 | 0.929 | 0.928 | 0.927 | 0.927 | 0.921 | 0.930 |
| $HF^+$ | 1.001 | 1.019 | 1.020 | 1.020 | 1.019 | 1.014 | 1.015 | 1.010 | 1.023 |
| $Na_2$ | 3.079 | 3.079 | 3.079 | 3.079 | 3.079 | 3.131 | 3.130 | 3.142 | 3.079 |
| NaH | 1.887 | 1.891 | 1.892 | 1.892 | 1.892 | 1.887 | 1.887 | 1.898 | 1.893 |
| NaF | 1.926 | 1.931 | 1.931 | 1.931 | 1.930 | 1.929 | 1.929 | 1.926 | 1.940 |
| NaCl | 2.361 | 2.361 | 2.361 | 2.361 | 2.361 | 2.358 | 2.358 | 2.365 | 2.367 |
| NaO | 2.052 | 2.059 | 2.059 | 2.059 | 2.059 | 2.055 | 2.056 | 2.056 | 2.070 |
| MgH | 1.730 | 1.750 | 1.751 | 1.751 | 1.751 | 1.735 | 1.736 | 1.745 | 1.757 |
| MgF | 1.750 | 1.775 | 1.774 | 1.774 | 1.773 | 1.771 | 1.771 | 1.766 | 1.784 |
| MgCl | 2.196 | 2.215 | 2.214 | 2.214 | 2.214 | 2.209 | 2.209 | 2.212 | 2.226 |
| MgO | 1.748 | 1.748 | 1.744 | 1.744 | 1.744 | 1.747 | 1.743 | 1.736 | 1.750 |
| $Al_2$ | 2.466 | 2.473 | 2.470 | 2.470 | 2.469 | 2.470 | 2.466 | 2.471 | 2.488 |
| AlH | 1.648 | 1.666 | 1.666 | 1.666 | 1.666 | 1.654 | 1.654 | 1.661 | 1.679 |
| AlF | 1.654 | 1.675 | 1.674 | 1.674 | 1.673 | 1.672 | 1.671 | 1.664 | 1.684 |
| AlCl | 2.130 | 2.150 | 2.149 | 2.149 | 2.149 | 2.143 | 2.143 | 2.145 | 2.163 |
| AlO | 1.618 | 1.633 | 1.629 | 1.629 | 1.629 | 1.631 | 1.628 | 1.619 | 1.633 |
| AlS | 2.029 | 2.042 | 2.040 | 2.040 | 2.039 | 2.038 | 2.035 | 2.031 | 2.049 |
| $Si_2$ | 2.246 | 2.155 | 2.157 | 2.157 | 2.156 | 2.149 | 2.152 | 2.152 | 2.287 |
| SiH | 1.520 | 1.538 | 1.537 | 1.538 | 1.538 | 1.527 | 1.526 | 1.530 | 1.545 |
| $SiH_4$ | 1.480 | 1.486 | 1.485 | 1.485 | 1.485 | 1.481 | 1.481 | 1.482 | 1.493 |
| SiF | 1.601 | 1.625 | 1.623 | 1.623 | 1.623 | 1.622 | 1.620 | 1.613 | 1.632 |
| $SiF_4$ | 1.553 | 1.574 | 1.572 | 1.572 | 1.572 | 1.572 | 1.571 | 1.564 | 1.580 |
| SiCl | 2.058 | 2.077 | 2.076 | 2.076 | 2.075 | 2.074 | 2.072 | 2.070 | 2.084 |
| $SiCl_4$ | 2.019 | 2.029 | 2.028 | 2.028 | 2.028 | 2.026 | 2.026 | 2.025 | 2.039 |
| SiN | 1.572 | 1.576 | 1.575 | 1.575 | 1.575 | 1.573 | 1.572 | 1.569 | 1.580 |
| SiO | 1.510 | 1.524 | 1.524 | 1.524 | 1.523 | 1.522 | 1.521 | 1.515 | 1.529 |
| SiS | 1.929 | 1.942 | 1.942 | 1.942 | 1.942 | 1.937 | 1.938 | 1.937 | 1.951 |
| $P_2$ | 1.893 | 1.896 | 1.897 | 1.897 | 1.897 | 1.891 | 1.893 | 1.891 | 1.905 |
| $P_4$ | 2.210 | 2.199 | 2.199 | 2.198 | 2.198 | 2.195 | 2.194 | 2.190 | 2.208 |
| PH | 1.421 | 1.436 | 1.435 | 1.436 | 1.435 | 1.427 | 1.427 | 1.427 | 1.440 |
| PF | 1.589 | 1.611 | 1.609 | 1.609 | 1.608 | 1.609 | 1.607 | 1.599 | 1.617 |
| PCl | 2.015 | 2.028 | 2.026 | 2.025 | 2.025 | 2.026 | 2.023 | 2.019 | 2.031 |
| PN | 1.491 | 1.495 | 1.496 | 1.496 | 1.495 | 1.492 | 1.493 | 1.487 | 1.500 |
| PO | 1.476 | 1.493 | 1.492 | 1.492 | 1.491 | 1.490 | 1.489 | 1.482 | 1.497 |
| $S_2$ | 1.889 | 1.906 | 1.905 | 1.905 | 1.904 | 1.904 | 1.902 | 1.896 | 1.912 |
| SH | 1.341 | 1.351 | 1.352 | 1.352 | 1.352 | 1.345 | 1.346 | 1.345 | 1.356 |
| SF | 1.601 | 1.621 | 1.618 | 1.618 | 1.617 | 1.620 | 1.616 | 1.605 | 1.622 |
| $SF_6$ | 1.561 | 1.589 | 1.585 | 1.586 | 1.585 | 1.588 | 1.584 | 1.576 | 1.596 |
| SO | 1.481 | 1.503 | 1.501 | 1.501 | 1.501 | 1.501 | 1.499 | 1.490 | 1.505 |
| $SO_3$ | 1.420 | 1.441 | 1.439 | 1.439 | 1.438 | 1.439 | 1.437 | 1.429 | 1.444 |
| $Cl_2$ | 1.988 | 2.013 | 2.009 | 2.009 | 2.008 | 2.012 | 2.008 | 1.996 | 2.008 |
| $Cl_2^+$ | 1.891 | 1.915 | 1.911 | 1.911 | 1.910 | 1.913 | 1.910 | 1.898 | 1.914 |
| HCl | 1.275 | 1.283 | 1.285 | 1.285 | 1.285 | 1.279 | 1.281 | 1.279 | 1.288 |
| $HCl^+$ | 1.315 | 1.327 | 1.329 | 1.329 | 1.329 | 1.320 | 1.322 | 1.321 | 1.333 |
| ClF | 1.628 | 1.655 | 1.651 | 1.651 | 1.651 | 1.654 | 1.650 | 1.636 | 1.652 |
| ClO | 1.570 | 1.594 | 1.589 | 1.589 | 1.588 | 1.595 | 1.589 | 1.575 | 1.583 |
| ME | | 0.012 | 0.013 | 0.013 | 0.011 | 0.008 | 0.008 | 0.005 | 0.018 |
| MAD | | 0.014 | 0.015 | 0.015 | 0.014 | 0.011 | 0.011 | 0.010 | 0.018 |

TABLE XI: Harmonic vibrational frequencies in $cm^{-1}$ for the T82-F molecular test set [8, 9] obtained with different approximate exchange-correlation functionals.

| Molecule | Exp. | X C | *rreg*TM *rreg*TM | *v1-sreg*TM *rreg*TM | *v2-sreg*TM *rreg*TM | *v3-sreg*TM *rreg*TM | *rreg*TM *PBE* | *v2-sreg*TM *PBE* | $r^2$SCAN $r^2$SCAN | *PBE* *PBE* |
|---|---|---|---|---|---|---|---|---|---|---|
| $H_2$ | 4401.20 | | 4387.64 | 4387.61 | 4387.61 | 4387.55 | 4423.31 | 4423.28 | 4429.67 | 4316.60 |
| $Li_2$ | 351.40 | | 328.66 | 329.72 | 329.64 | 329.92 | 338.35 | 338.47 | 332.37 | 329.83 |
| LiH | 1405.70 | | 1384.23 | 1383.65 | 1383.55 | 1383.36 | 1411.41 | 1411.80 | 1394.28 | 1377.44 |
| LiF | 910.60 | | 891.62 | 892.88 | 892.81 | 893.16 | 905.41 | 906.59 | 904.77 | 894.04 |
| LiCl | 643.00 | | 638.40 | 639.70 | 639.72 | 640.09 | 649.50 | 650.72 | 642.66 | 644.19 |
| LiO | 814.60 | | 798.41 | 798.95 | 798.89 | 799.31 | 813.86 | 813.97 | 810.73 | 797.92 |
| LiNa | 256.80 | | 254.54 | 249.03 | 249.29 | 249.62 | 251.78 | 245.86 | 246.33 | 245.92 |
| $Be_2$ | 267.90 | | 339.05 | 323.64 | 323.90 | 327.12 | 351.44 | 352.32 | 327.20 | 347.20 |
| BeH | 2060.80 | | 1985.19 | 1984.83 | 1984.70 | 1984.22 | 2040.86 | 2040.48 | 2009.73 | 1974.63 |
| $BeH^+$ | 2221.70 | | 2146.42 | 2149.42 | 2149.13 | 2148.95 | 2184.24 | 2186.90 | 2203.03 | 2109.72 |
| BeF | 1247.40 | | 1203.54 | 1206.17 | 1206.13 | 1206.60 | 1211.30 | 1213.90 | 1222.55 | 1196.15 |
| BeCl | 846.70 | | 812.04 | 812.50 | 812.56 | 813.26 | 821.58 | 821.89 | 816.44 | 809.36 |
| BeO | 1487.30 | | 1463.82 | 1468.96 | 1468.96 | 1470.20 | 1474.61 | 1479.45 | 1508.31 | 1455.69 |
| BeS | 997.90 | | 984.82 | 988.50 | 988.72 | 989.85 | 991.92 | 995.86 | 1008.22 | 975.83 |
| $B_2$ | 1051.30 | | 997.04 | 1008.78 | 1010.37 | 1009.68 | 997.94 | 1013.61 | 1012.77 | 1011.60 |
| BH | 2366.90 | | 2274.37 | 2272.63 | 2273.02 | 2270.34 | 2347.26 | 2346.24 | 2301.01 | 2245.71 |
| BF | 1402.10 | | 1371.26 | 1374.12 | 1373.97 | 1374.96 | 1381.29 | 1383.48 | 1398.46 | 1354.73 |
| BCl | 840.30 | | 823.70 | 816.39 | 816.44 | 817.46 | 839.54 | 831.12 | 826.55 | 810.20 |
| BN | 1514.60 | | 1534.84 | 1524.21 | 1524.17 | 1526.35 | 1556.10 | 1544.90 | 1570.16 | 1513.24 |
| BO | 1885.70 | | 1853.12 | 1854.69 | 1854.60 | 1856.23 | 1867.82 | 1868.82 | 1896.33 | 1844.00 |
| BS | 1180.20 | | 1170.12 | 1169.79 | 1170.51 | 1171.89 | 1180.66 | 1180.60 | 1195.46 | 1161.49 |
| $C_2$ | 1854.70 | | 1846.34 | 1857.32 | 1860.38 | 1862.84 | 1845.50 | 1860.90 | 1891.01 | 1857.11 |
| CH | 2858.50 | | 2738.12 | 2725.24 | 2726.40 | 2727.85 | 2817.65 | 2808.77 | 2803.97 | 2730.18 |
| CF | 1308.10 | | 1254.54 | 1262.65 | 1263.46 | 1264.39 | 1258.56 | 1266.11 | 1297.42 | 1257.32 |
| CN | 2068.60 | | 2093.37 | 2096.91 | 2098.35 | 2100.44 | 2105.00 | 2108.94 | 2149.60 | 2093.57 |
| CO | 2169.80 | | 2153.95 | 2148.45 | 2148.72 | 2150.60 | 2167.73 | 2162.13 | 2195.55 | 2129.62 |
| $CO^+$ | 2214.20 | | 2209.94 | 2213.52 | 2214.18 | 2216.64 | 2224.73 | 2228.25 | 2277.95 | 2202.58 |
| CP | 1239.70 | | 1262.02 | 1263.72 | 1264.31 | 1265.84 | 1270.35 | 1271.96 | 1286.41 | 1250.18 |
| CS | 1285.20 | | 1285.03 | 1276.40 | 1277.34 | 1278.70 | 1299.05 | 1290.86 | 1304.75 | 1263.69 |
| $N_2$ | 2358.60 | | 2384.46 | 2373.02 | 2374.48 | 2376.59 | 2402.25 | 2391.08 | 2432.68 | 2353.66 |
| $N_2^+$ | 2207.00 | | 2263.01 | 2267.89 | 2270.16 | 2272.37 | 2272.60 | 2279.75 | 2326.82 | 2264.91 |
| NH | 3282.30 | | 3176.96 | 3182.65 | 3183.72 | 3178.92 | 3242.12 | 3247.86 | 3246.50 | 3171.82 |
| NF | 1141.40 | | 1115.21 | 1136.97 | 1137.14 | 1137.98 | 1116.17 | 1137.95 | 1171.33 | 1128.53 |
| NCl | 828.00 | | 818.88 | 824.79 | 826.06 | 826.57 | 818.83 | 825.33 | 836.47 | 835.85 |
| NO | 1904.20 | | 1897.34 | 1899.99 | 1901.66 | 1903.83 | 1907.39 | 1911.17 | 1959.47 | 1892.16 |
| $NO^+$ | 2376.40 | | 2395.45 | 2387.78 | 2389.33 | 2391.71 | 2413.75 | 2406.85 | 2456.14 | 2363.83 |
| NS | 1218.70 | | 1219.33 | 1222.56 | 1223.24 | 1224.76 | 1227.34 | 1230.68 | 1254.42 | 1213.17 |
| $O_2$ | 1580.20 | | 1554.74 | 1563.71 | 1565.23 | 1566.68 | 1557.62 | 1568.15 | 1624.96 | 1555.90 |
| $O_2^+$ | 1904.80 | | 1941.06 | 1947.67 | 1949.39 | 1951.56 | 1949.82 | 1958.07 | 2026.58 | 1931.33 |
| OH | 3737.80 | | 3627.98 | 3622.10 | 3622.55 | 3627.47 | 3654.09 | 3648.88 | 3718.29 | 3602.70 |
| $OH^+$ | 3113.40 | | 2995.45 | 2992.68 | 2992.91 | 2994.57 | 3056.99 | 3054.84 | 3060.89 | 2953.36 |
| $F_2$ | 916.60 | | 1002.19 | 1007.52 | 1006.95 | 1006.40 | 1003.89 | 1007.99 | 1048.14 | 997.29 |
| $F_2^+$ | 1073.30 | | 1161.56 | 1167.18 | 1166.73 | 1167.64 | 1163.55 | 1168.53 | 1219.83 | 1151.83 |
| HF | 4138.30 | | 3981.32 | 3992.67 | 3992.60 | 3997.21 | 3994.59 | 4005.79 | 4093.34 | 3977.20 |
| $HF^+$ | 3090.50 | | 2950.45 | 2945.42 | 2945.42 | 2949.03 | 2989.28 | 2983.36 | 3024.75 | 2910.03 |
| $Na_2$ | 159.10 | | 158.26 | 159.67 | 159.77 | 159.82 | 149.71 | 152.12 | 155.29 | 158.96 |
| NaH | 1172.20 | | 1158.49 | 1157.40 | 1157.37 | 1157.21 | 1177.48 | 1178.33 | 1167.88 | 1143.28 |
| NaF | 535.70 | | 532.82 | 533.51 | 533.49 | 533.71 | 533.88 | 534.62 | 539.36 | 519.85 |

(continued)

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| NaO | 492.30 | 481.58 | 481.60 | 481.59 | 481.87 | 484.27 | 484.31 | 488.05 | 466.16 |
| MgH | 1495.20 | 1426.67 | 1427.09 | 1426.83 | 1426.73 | 1491.74 | 1491.76 | 1461.59 | 1409.21 |
| $MgH^+$ | 1699.10 | 1681.16 | 1681.93 | 1681.72 | 1681.62 | 1711.13 | 1711.70 | 1720.88 | 1642.69 |
| MgO | 784.80 | 806.52 | 817.18 | 817.05 | 817.70 | 805.59 | 815.84 | 837.42 | 803.21 |
| MgS | 528.70 | 534.86 | 541.36 | 541.32 | 541.94 | 534.79 | 541.67 | 550.24 | 526.22 |
| $Al_2$ | 350.00 | 352.59 | 354.54 | 355.01 | 355.49 | 352.68 | 356.04 | 355.77 | 341.93 |
| AlH | 1682.60 | 1627.00 | 1629.99 | 1629.37 | 1628.22 | 1680.51 | 1682.04 | 1646.51 | 1585.99 |
| AlF | 802.30 | 769.35 | 771.59 | 771.53 | 772.08 | 774.87 | 776.90 | 788.75 | 747.66 |
| AlCl | 481.30 | 469.23 | 471.00 | 470.88 | 471.32 | 474.81 | 476.30 | 475.87 | 458.80 |
| AlO | 979.20 | 951.23 | 964.97 | 964.59 | 965.60 | 951.57 | 965.69 | 992.26 | 956.88 |
| AlS | 617.10 | 606.76 | 614.05 | 614.07 | 615.03 | 610.28 | 618.05 | 630.55 | 600.43 |
| $Si_2$ | 511.00 | 554.83 | 553.56 | 554.00 | 554.97 | 559.61 | 558.72 | 564.20 | 483.24 |
| SiH | 2041.80 | 1981.19 | 1984.29 | 1983.17 | 1982.79 | 2041.66 | 2044.43 | 2020.24 | 1951.71 |
| $SiH^+$ | 2157.20 | 2093.81 | 2098.33 | 2097.95 | 2096.81 | 2140.07 | 2144.42 | 2119.64 | 2047.83 |
| SiF | 857.20 | 825.32 | 829.84 | 829.54 | 830.28 | 829.21 | 834.03 | 847.30 | 807.65 |
| SiCl | 535.60 | 520.92 | 523.51 | 523.20 | 523.83 | 524.34 | 527.70 | 529.27 | 515.10 |
| SiN | 1151.40 | 1160.86 | 1165.03 | 1164.84 | 1165.80 | 1165.76 | 1169.33 | 1179.68 | 1150.13 |
| SiO | 1241.50 | 1217.05 | 1219.35 | 1219.16 | 1220.13 | 1225.91 | 1227.77 | 1247.89 | 1196.56 |
| SiS | 749.60 | 741.01 | 741.35 | 741.53 | 742.31 | 749.07 | 749.27 | 753.33 | 726.42 |
| $P_2$ | 780.80 | 798.51 | 797.35 | 797.87 | 798.72 | 808.14 | 805.83 | 813.84 | 782.42 |
| $P_2{}^+$ | 672.20 | 693.34 | 690.24 | 690.94 | 691.85 | 703.11 | 700.45 | 707.78 | 674.31 |
| PH | 2365.20 | 2313.07 | 2314.07 | 2314.35 | 2314.98 | 2369.48 | 2368.74 | 2367.90 | 2288.59 |
| PF | 846.80 | 822.79 | 828.46 | 827.94 | 828.66 | 826.47 | 831.54 | 846.90 | 811.02 |
| PCl | 551.40 | 540.49 | 542.78 | 542.79 | 543.19 | 542.39 | 544.09 | 550.12 | 538.06 |
| PN | 1337.20 | 1361.57 | 1358.90 | 1358.82 | 1360.18 | 1373.75 | 1370.51 | 1390.71 | 1339.51 |
| PO | 1233.30 | 1214.19 | 1219.85 | 1219.51 | 1220.80 | 1221.97 | 1227.10 | 1250.59 | 1200.39 |
| $S_2$ | 725.60 | 709.90 | 713.89 | 714.98 | 715.74 | 713.63 | 718.56 | 732.65 | 701.88 |
| SO | 1149.20 | 1117.20 | 1124.33 | 1124.27 | 1125.55 | 1121.43 | 1128.30 | 1159.28 | 1110.40 |
| $Cl_2$ | 559.70 | 538.45 | 541.10 | 541.26 | 541.59 | 539.92 | 542.98 | 555.49 | 540.40 |
| $Cl_2{}^+$ | 645.60 | 626.46 | 629.64 | 630.10 | 630.62 | 627.93 | 631.30 | 649.26 | 624.21 |
| HCl | 2990.90 | 2937.18 | 2920.15 | 2922.44 | 2926.04 | 2969.46 | 2953.90 | 2981.86 | 2901.24 |
| $HCl^+$ | 2673.70 | 2600.18 | 2581.42 | 2583.30 | 2586.47 | 2653.39 | 2635.95 | 2643.90 | 2571.65 |
| ClF | 786.10 | 760.96 | 764.79 | 764.77 | 765.21 | 762.46 | 766.26 | 791.24 | 760.84 |
| ClO | 853.80 | 841.27 | 849.04 | 849.56 | 850.23 | 836.64 | 844.85 | 872.53 | 862.59 |
| ME | | -21.00 | -19.62 | -19.28 | -18.35 | -4.67 | -2.87 | 11.34 | -33.78 |
| MAD | | 35.57 | 34.28 | 34.27 | 34.12 | 25.18 | 24.14 | 30.90 | 43.61 |

## VI. SOLID TEST SET RESULTS

Here we provide the solid-by-solid tabulation for the band gaps (21 systems), equilibrium lattice constants and cohesive energies (55 solids), and bulk moduli (44 cubic solids) for *rreg*TM compared with *sreg*TM, r$^2$SCAN, and PBE.

TABLE XII. Band Gap ($eV$) of 21 insulators and semiconductors. Experimental lattice parameters were used with all functionals. Experimental values Exptl. and lattice constants are from Ref. [12].

| Solid | Exp. | X<br>C | *rreg*TM<br>*rreg*TM | *v1-sreg*TM<br>*rreg*TM | *v2-sreg*TM<br>*rreg*TM | *v3-sreg*TM<br>*rreg*TM | *rreg*TM<br>*PBE* | *v2-sreg*TM<br>*PBE* | r$^2$SCAN<br>r$^2$SCAN | *PBE*<br>*PBE* |
|---|---|---|---|---|---|---|---|---|---|---|
| C | 5.50 | | 4.48 | 4.13 | 4.14 | 4.16 | 4.76 | 4.42 | 4.32 | 4.13 |
| Si | 1.17 | | 0.82 | 0.63 | 0.63 | 0.65 | 1.06 | 0.88 | 0.78 | 0.58 |
| Ge | 0.74 | | 0.33 | 0.38 | 0.39 | 0.41 | 0.37 | 0.44 | 0.50 | 0.09 |
| SiC | 2.42 | | 1.52 | 1.44 | 1.46 | 1.48 | 1.61 | 1.54 | 1.75 | 1.38 |
| BN | 6.36 | | 4.72 | 4.57 | 4.59 | 4.62 | 4.87 | 4.73 | 5.00 | 4.48 |
| BP | 2.10 | | 1.50 | 1.28 | 1.28 | 1.30 | 1.71 | 1.50 | 1.45 | 1.24 |
| AlN | 4.90 | | 3.46 | 3.48 | 3.50 | 3.52 | 3.49 | 3.52 | 3.97 | 3.35 |
| AlP | 2.50 | | 1.79 | 1.70 | 1.71 | 1.73 | 1.93 | 1.84 | 1.92 | 1.59 |
| AlAs | 2.23 | | 1.63 | 1.59 | 1.60 | 1.61 | 1.70 | 1.66 | 1.80 | 1.44 |
| GaN | 3.28 | | 1.69 | 1.76 | 1.77 | 1.79 | 1.68 | 1.76 | 2.19 | 1.74 |
| GaP | 2.35 | | 1.68 | 1.66 | 1.67 | 1.69 | 1.76 | 1.73 | 1.89 | 1.62 |
| GaAs | 1.52 | | 0.93 | 1.00 | 1.00 | 1.02 | 0.99 | 1.07 | 1.09 | 0.61 |
| InP | 1.42 | | 0.96 | 0.99 | 0.99 | 1.01 | 1.04 | 1.07 | 1.18 | 0.75 |
| InAs | 0.42 | | 0.11 | 0.17 | 0.18 | 0.19 | 0.15 | 0.22 | 0.25 | 0.00 |
| InSb | 0.24 | | 0.18 | 0.23 | 0.24 | 0.25 | 0.22 | 0.28 | 0.27 | 0.00 |
| LiH | 4.94 | | 3.34 | 3.33 | 3.34 | 3.34 | 3.69 | 3.69 | 3.72 | 3.07 |
| LiF | 14.20 | | 9.24 | 9.30 | 9.31 | 9.32 | 9.21 | 9.28 | 10.19 | 9.20 |
| LiCl | 9.40 | | 6.77 | 6.78 | 6.79 | 6.80 | 6.85 | 6.87 | 7.31 | 6.41 |
| NaF | 11.50 | | 6.25 | 6.32 | 6.32 | 6.33 | 6.25 | 6.33 | 7.21 | 6.37 |
| NaCl | 8.50 | | 5.36 | 5.39 | 5.39 | 5.41 | 5.44 | 5.48 | 5.98 | 5.19 |
| MgO | 7.83 | | 4.98 | 5.04 | 5.05 | 5.07 | 4.98 | 5.05 | 5.65 | 4.77 |
| ME | | | -1.52 | -1.54 | -1.53 | -1.52 | -1.42 | -1.44 | -1.20 | -1.69 |
| MAD | | | 1.52 | 1.54 | 1.53 | 1.52 | 1.42 | 1.44 | 1.20 | 1.69 |

TABLE XIII. Equilibrium lattice constants, $a_0(\AA)$ comparisons of 55 solids. Experimental values Exptl. are from Ref. [10], include zero-point effects.

| Solid | Exp. | X<br>C | *rreg*TM<br>*rreg*TM | *v1-sreg*TM<br>*rreg*TM | *v2-sreg*TM<br>*rreg*TM | *v3-sreg*TM<br>*rreg*TM | *rreg*TM<br>*PBE* | *v2-sreg*TM<br>*PBE* | r$^2$SCAN<br>r$^2$SCAN | *PBE*<br>*PBE* |
|---|---|---|---|---|---|---|---|---|---|---|
| C | 3.553 | | 3.560 | 3.565 | 3.565 | 3.565 | 3.555 | 3.560 | 3.562 | 3.572 |
| Si | 5.421 | | 5.425 | 5.430 | 5.430 | 5.430 | 5.417 | 5.420 | 5.440 | 5.469 |
| Ge | 5.644 | | 5.693 | 5.698 | 5.700 | 5.701 | 5.680 | 5.687 | 5.681 | 5.782 |
| Sn | 6.477 | | 6.545 | 6.555 | 6.559 | 6.561 | 6.528 | 6.542 | 6.565 | 6.653 |
| SiC | 4.346 | | 4.356 | 4.352 | 4.353 | 4.352 | 4.352 | 4.347 | 4.355 | 4.379 |
| BN | 3.592 | | 3.615 | 3.617 | 3.618 | 3.617 | 3.609 | 3.612 | 3.614 | 3.626 |
| BP | 4.525 | | 4.526 | 4.530 | 4.530 | 4.530 | 4.521 | 4.523 | 4.533 | 4.547 |
| AlN | 4.368 | | 4.374 | 4.372 | 4.372 | 4.371 | 4.367 | 4.366 | 4.368 | 4.402 |
| AlP | 5.451 | | 5.463 | 5.465 | 5.466 | 5.465 | 5.454 | 5.456 | 5.472 | 5.506 |
| AlAs | 5.649 | | 5.674 | 5.672 | 5.674 | 5.674 | 5.667 | 5.665 | 5.677 | 5.733 |
| GaN | 4.520 | | 4.560 | 4.557 | 4.557 | 4.557 | 4.555 | 4.552 | 4.527 | 4.589 |
| GaP | 5.439 | | 5.487 | 5.487 | 5.487 | 5.487 | 5.480 | 5.479 | 5.467 | 5.534 |
| GaAs | 5.640 | | 5.684 | 5.688 | 5.690 | 5.691 | 5.673 | 5.679 | 5.672 | 5.762 |
| InP | 5.858 | | 5.951 | 5.949 | 5.950 | 5.950 | 5.943 | 5.941 | 5.947 | 6.001 |
| InAs | 6.047 | | 6.128 | 6.132 | 6.135 | 6.136 | 6.115 | 6.122 | 6.131 | 6.211 |
| InSb | 6.468 | | 6.548 | 6.558 | 6.561 | 6.563 | 6.533 | 6.546 | 6.569 | 6.647 |
| LiH | 3.979 | | 3.983 | 3.984 | 3.986 | 3.986 | 3.940 | 3.944 | 4.012 | 4.016 |
| LiF | 3.972 | | 3.990 | 3.992 | 3.993 | 3.992 | 3.969 | 3.971 | 3.994 | 4.071 |
| LiCl | 5.070 | | 5.078 | 5.080 | 5.082 | 5.081 | 5.044 | 5.047 | 5.111 | 5.153 |
| NaF | 4.582 | | 4.497 | 4.501 | 4.501 | 4.501 | 4.491 | 4.495 | 4.503 | 4.632 |
| NaCl | 5.569 | | 5.504 | 5.508 | 5.509 | 5.509 | 5.489 | 5.495 | 5.545 | 5.655 |
| MgO | 4.189 | | 4.209 | 4.206 | 4.207 | 4.205 | 4.202 | 4.200 | 4.196 | 4.248 |
| Li | 3.443 | | 3.432 | 3.433 | 3.434 | 3.434 | 3.401 | 3.403 | 3.479 | 3.439 |
| Na | 4.214 | | 4.113 | 4.117 | 4.119 | 4.120 | 4.111 | 4.118 | 4.200 | 4.193 |
| K | 5.212 | | 5.199 | 5.203 | 5.207 | 5.209 | 5.202 | 5.213 | 5.350 | 5.286 |
| Rb | 5.577 | | 5.546 | 5.554 | 5.559 | 5.560 | 5.572 | 5.585 | 5.751 | 5.669 |
| Cs | 6.039 | | 6.044 | 6.057 | 6.063 | 6.067 | 6.063 | 6.083 | 6.271 | 6.161 |
| Ca | 5.556 | | 5.484 | 5.473 | 5.475 | 5.474 | 5.484 | 5.482 | 5.574 | 5.525 |
| Ba | 5.002 | | 4.988 | 4.994 | 4.999 | 5.002 | 4.990 | 5.002 | 5.077 | 5.030 |
| Sr | 6.040 | | 5.987 | 5.984 | 5.988 | 5.988 | 5.989 | 5.994 | 6.101 | 6.027 |
| Al | 4.018 | | 3.986 | 3.983 | 3.982 | 3.981 | 3.980 | 3.975 | 3.988 | 4.040 |
| Fe | 2.853 | | 2.799 | 2.805 | 2.807 | 2.808 | 2.798 | 2.806 | 2.865 | 2.829 |
| Co | 3.524 | | 3.501 | 3.494 | 3.497 | 3.498 | 3.502 | 3.500 | 3.514 | 3.517 |
| Ni | 3.508 | | 3.476 | 3.477 | 3.479 | 3.480 | 3.470 | 3.473 | 3.479 | 3.518 |
| Sc | 3.270 | | 3.235 | 3.233 | 3.235 | 3.235 | 3.234 | 3.234 | 3.260 | 3.249 |
| Y | 3.594 | | 3.588 | 3.591 | 3.593 | 3.594 | 3.587 | 3.595 | 3.623 | 3.592 |
| Ti | 2.915 | | 2.878 | 2.877 | 2.879 | 2.879 | 2.876 | 2.877 | 2.887 | 2.893 |
| Zr | 3.198 | | 3.205 | 3.203 | 3.206 | 3.206 | 3.204 | 3.205 | 3.215 | 3.210 |
| Hf | 3.151 | | 3.129 | 3.132 | 3.134 | 3.135 | 3.127 | 3.132 | 3.141 | 3.158 |
| V | 3.021 | | 2.964 | 2.964 | 2.966 | 2.966 | 2.962 | 2.963 | 2.965 | 2.978 |
| Nb | 3.294 | | 3.319 | 3.316 | 3.318 | 3.319 | 3.317 | 3.317 | 3.320 | 3.322 |
| Ta | 3.299 | | 3.283 | 3.285 | 3.287 | 3.288 | 3.280 | 3.284 | 3.290 | 3.309 |
| Mo | 3.141 | | 3.139 | 3.139 | 3.141 | 3.141 | 3.136 | 3.138 | 3.144 | 3.151 |
| W | 3.160 | | 3.151 | 3.152 | 3.154 | 3.154 | 3.148 | 3.151 | 3.156 | 3.172 |
| Tc | 2.716 | | 2.711 | 2.711 | 2.713 | 2.713 | 2.708 | 2.710 | 2.716 | 2.725 |
| Re | 2.744 | | 2.746 | 2.747 | 2.749 | 2.749 | 2.744 | 2.747 | 2.750 | 2.764 |
| Ru | 2.669 | | 2.669 | 2.671 | 2.673 | 2.673 | 2.667 | 2.670 | 2.672 | 2.683 |
| Os | 2.699 | | 2.703 | 2.705 | 2.706 | 2.707 | 2.701 | 2.704 | 2.708 | 2.723 |
| Rh | 3.794 | | 3.800 | 3.803 | 3.806 | 3.806 | 3.796 | 3.801 | 3.804 | 3.824 |
| Ir | 3.831 | | 3.844 | 3.848 | 3.850 | 3.851 | 3.840 | 3.846 | 3.852 | 3.872 |
| Pd | 3.876 | | 3.902 | 3.905 | 3.909 | 3.910 | 3.896 | 3.903 | 3.912 | 3.939 |
| Pt | 3.913 | | 3.933 | 3.937 | 3.941 | 3.942 | 3.927 | 3.935 | 3.943 | 3.968 |
| Cu | 3.595 | | 3.569 | 3.574 | 3.577 | 3.578 | 3.563 | 3.570 | 3.582 | 3.634 |
| Ag | 4.062 | | 4.082 | 4.087 | 4.092 | 4.094 | 4.075 | 4.084 | 4.108 | 4.147 |
| Au | 4.062 | | 4.108 | 4.114 | 4.118 | 4.120 | 4.100 | 4.111 | 4.128 | 4.156 |
| ME | | | 0.000 | 0.002 | 0.004 | 0.005 | -0.006 | -0.002 | 0.026 | 0.046 |
| MAD | | | 0.029 | 0.030 | 0.031 | 0.031 | 0.028 | 0.029 | 0.037 | 0.053 |

TABLE XIV. Cohesive energies, $E_{coh}(eV/atom)$ of 55 solids. Experimental values Exptl. are from Ref. [10], include zero-point effects.

| Solid | Exp. | X C | *rreg*TM *rreg*TM | *v1-sreg*TM *rreg*TM | *v2-sreg*TM *rreg*TM | *v3-sreg*TM *rreg*TM | *rreg*TM *PBE* | *v2-sreg*TM *PBE* | r$^2$SCAN r$^2$SCAN | *PBE* *PBE* |
|---|---|---|---|---|---|---|---|---|---|---|
| C | 7.550 | | 7.552 | 7.524 | 7.528 | 7.539 | 7.567 | 7.527 | 7.467 | 7.714 |
| Si | 4.680 | | 4.671 | 4.640 | 4.642 | 4.650 | 4.746 | 4.696 | 4.675 | 4.561 |
| Ge | 3.890 | | 3.923 | 3.892 | 3.889 | 3.883 | 3.946 | 3.912 | 3.891 | 3.725 |
| Sn | 3.160 | | 3.409 | 3.360 | 3.356 | 3.348 | 3.431 | 3.377 | 3.295 | 3.200 |
| SiC | 6.480 | | 6.423 | 6.468 | 6.462 | 6.470 | 6.434 | 6.465 | 6.432 | 6.408 |
| BN | 6.760 | | 6.919 | 6.912 | 6.906 | 6.914 | 6.916 | 6.894 | 6.788 | 6.936 |
| BP | 5.140 | | 5.339 | 5.275 | 5.277 | 5.287 | 5.383 | 5.302 | 5.281 | 5.293 |
| AlN | 5.850 | | 5.891 | 5.930 | 5.922 | 5.926 | 5.890 | 5.920 | 5.809 | 5.711 |
| AlP | 4.320 | | 4.287 | 4.275 | 4.270 | 4.276 | 4.337 | 4.308 | 4.249 | 4.093 |
| AlAs | 3.820 | | 3.886 | 3.879 | 3.874 | 3.875 | 3.903 | 3.886 | 3.867 | 3.693 |
| GaN | 4.550 | | 4.615 | 4.628 | 4.620 | 4.619 | 4.633 | 4.637 | 4.465 | 4.385 |
| GaP | 3.610 | | 3.698 | 3.690 | 3.685 | 3.685 | 3.732 | 3.715 | 3.642 | 3.478 |
| GaAs | 3.340 | | 3.406 | 3.376 | 3.372 | 3.366 | 3.429 | 3.395 | 3.328 | 3.161 |
| InP | 3.470 | | 3.358 | 3.354 | 3.348 | 3.346 | 3.382 | 3.371 | 3.245 | 3.123 |
| InAs | 3.080 | | 3.154 | 3.119 | 3.114 | 3.108 | 3.175 | 3.135 | 3.026 | 2.893 |
| InSb | 2.810 | | 2.881 | 2.835 | 2.830 | 2.823 | 2.901 | 2.850 | 2.729 | 2.650 |
| LiH | 2.490 | | 2.450 | 2.449 | 2.447 | 2.446 | 2.474 | 2.470 | 2.420 | 2.348 |
| LiF | 4.460 | | 4.339 | 4.391 | 4.388 | 4.390 | 4.290 | 4.339 | 4.395 | 4.321 |
| LiCl | 3.590 | | 3.482 | 3.518 | 3.516 | 3.517 | 3.435 | 3.469 | 3.467 | 3.352 |
| NaF | 3.970 | | 3.923 | 3.973 | 3.970 | 3.971 | 3.880 | 3.927 | 3.992 | 3.860 |
| NaCl | 3.340 | | 3.258 | 3.293 | 3.291 | 3.292 | 3.228 | 3.260 | 3.260 | 3.088 |
| MgO | 5.200 | | 5.139 | 5.183 | 5.177 | 5.182 | 5.155 | 5.192 | 5.249 | 4.998 |
| Li | 1.670 | | 1.638 | 1.641 | 1.641 | 1.641 | 1.591 | 1.595 | 1.569 | 1.600 |
| Na | 1.120 | | 1.140 | 1.137 | 1.134 | 1.133 | 1.124 | 1.118 | 1.041 | 1.038 |
| K | 0.940 | | 0.959 | 0.957 | 0.954 | 0.953 | 0.958 | 0.952 | 0.841 | 0.857 |
| Rb | 0.860 | | 0.858 | 0.853 | 0.849 | 0.847 | 0.877 | 0.868 | 0.734 | 0.760 |
| Cs | 0.810 | | 0.813 | 0.807 | 0.803 | 0.801 | 0.821 | 0.812 | 0.661 | 0.693 |
| Ca | 1.870 | | 1.898 | 1.930 | 1.923 | 1.920 | 2.025 | 2.052 | 1.917 | 1.846 |
| Ba | 1.910 | | 1.968 | 1.958 | 1.947 | 1.944 | 2.099 | 2.078 | 1.817 | 1.703 |
| Sr | 1.730 | | 1.855 | 1.843 | 1.835 | 1.833 | 2.000 | 1.981 | 1.786 | 1.604 |
| Al | 3.430 | | 3.653 | 3.662 | 3.656 | 3.652 | 3.662 | 3.667 | 3.609 | 3.442 |
| Fe | 4.300 | | 5.064 | 5.153 | 5.121 | 5.100 | 5.102 | 5.166 | 4.635 | 4.871 |
| Co | 4.420 | | 5.023 | 5.269 | 5.242 | 5.214 | 5.055 | 5.360 | 4.871 | 5.165 |
| Ni | 4.480 | | 5.127 | 5.392 | 5.132 | 5.105 | 5.438 | 5.193 | 4.645 | 4.732 |
| Sc | 3.930 | | 4.277 | 4.349 | 4.337 | 4.329 | 4.635 | 4.410 | 4.017 | 4.142 |
| Y | 4.390 | | 4.405 | 4.402 | 4.386 | 4.377 | 4.523 | 4.505 | 4.014 | 4.100 |
| Ti | 4.880 | | 5.158 | 5.381 | 5.364 | 5.353 | 5.166 | 5.372 | 5.060 | 5.442 |
| Zr | 6.270 | | 6.322 | 6.007 | 6.001 | 5.940 | 6.376 | 6.049 | 4.378 | 5.344 |
| Hf | 6.460 | | 6.948 | 6.880 | 6.854 | 6.838 | 7.087 | 6.994 | 6.434 | 6.455 |
| V | 5.350 | | 6.331 | 5.637 | 5.606 | 5.583 | 5.654 | 5.623 | 4.660 | 6.520 |
| Nb | 7.600 | | 7.269 | 7.205 | 7.168 | 7.146 | 7.299 | 7.204 | 6.361 | 6.919 |
| Ta | 8.130 | | 8.952 | 8.845 | 8.807 | 8.783 | 9.087 | 8.942 | 8.251 | 8.314 |
| Mo | 6.860 | | 6.830 | 6.721 | 6.676 | 6.648 | 6.875 | 6.720 | 5.690 | 6.351 |
| W | 8.940 | | 9.205 | 9.052 | 9.017 | 8.985 | 9.279 | 9.090 | 8.067 | 8.485 |
| Tc | 6.880 | | 7.479 | 7.353 | 7.299 | 7.323 | 7.502 | 7.360 | 6.337 | 6.971 |
| Re | 8.050 | | 8.654 | 8.490 | 8.440 | 8.403 | 8.783 | 8.568 | 7.514 | 7.815 |
| Ru | 6.770 | | 6.997 | 7.005 | 6.954 | 6.922 | 7.028 | 6.987 | 6.338 | 6.773 |
| Os | 8.200 | | 9.099 | 8.926 | 8.872 | 8.834 | 9.223 | 8.994 | 8.072 | 8.356 |
| Rh | 5.780 | | 6.116 | 6.096 | 6.050 | 6.018 | 6.150 | 6.085 | 5.826 | 5.748 |
| Ir | 6.990 | | 8.002 | 7.832 | 7.783 | 7.745 | 8.050 | 7.851 | 7.142 | 7.494 |
| Pd | 3.930 | | 4.596 | 4.503 | 4.470 | 4.444 | 4.652 | 4.524 | 4.163 | 3.738 |
| Pt | 5.870 | | 6.303 | 6.172 | 6.130 | 6.101 | 6.386 | 6.212 | 5.716 | 5.531 |
| Cu | 3.510 | | 4.306 | 4.227 | 4.198 | 4.181 | 4.370 | 4.262 | 3.855 | 3.479 |
| Ag | 2.960 | | 3.261 | 3.193 | 3.168 | 3.152 | 3.310 | 3.217 | 2.873 | 2.511 |
| Au | 3.830 | | 3.820 | 3.730 | 3.702 | 3.681 | 3.883 | 3.764 | 3.417 | 3.033 |
| ME | | | 0.212 | 0.18 | 0.159 | 0.148 | 0.248 | 0.199 | -0.134 | -0.070 |
| MAD | | | 0.251 | 0.232 | 0.216 | 0.210 | 0.288 | 0.251 | 0.238 | 0.252 |

TABLE XV. Bulk modulus, $B_0(GPa)$ of 44 cubic solids. Experimental values Exptl. are from Ref. [11], these values were obtained by subtracting the zero-point phonon effect from the experimental zero-temperature values.

| Solid | Exp. | X<br>C | *rreg*TM<br>*rreg*TM | *v1-sreg*TM<br>*rreg*TM | *v2-sreg*TM<br>*rreg*TM | *v3-sreg*TM<br>*rreg*TM | *rreg*TM<br>*PBE* | *v2-sreg*TM<br>*PBE* | r$^2$SCAN<br>r$^2$SCAN | *PBE*<br>*PBE* |
|---|---|---|---|---|---|---|---|---|---|---|
| C | 454.700 | | 449.794 | 439.039 | 439.805 | 440.565 | 459.618 | 449.531 | 449.244 | 433.061 |
| Si | 101.300 | | 98.870 | 95.336 | 95.389 | 95.712 | 103.557 | 100.463 | 97.272 | 88.798 |
| Ge | 79.400 | | 70.014 | 69.709 | 69.611 | 69.619 | 72.193 | 71.784 | 73.095 | 59.083 |
| Sn | 42.800 | | 43.263 | 42.780 | 42.673 | 42.617 | 44.541 | 43.929 | 43.526 | 36.172 |
| SiC | 229.100 | | 225.815 | 224.577 | 224.220 | 224.633 | 229.867 | 228.388 | 226.927 | 212.361 |
| BN | 410.200 | | 387.268 | 383.780 | 383.296 | 384.044 | 394.985 | 390.743 | 389.901 | 372.412 |
| BP | 168.000 | | 171.053 | 166.161 | 166.357 | 166.754 | 176.357 | 171.680 | 170.052 | 161.851 |
| AlN | 206.000 | | 206.487 | 207.245 | 207.037 | 207.479 | 209.598 | 210.108 | 212.380 | 193.670 |
| AlP | 87.400 | | 91.687 | 90.035 | 89.942 | 90.195 | 94.901 | 93.076 | 91.095 | 82.678 |
| AlAs | 75.000 | | 76.308 | 75.745 | 75.557 | 75.670 | 78.332 | 77.566 | 76.387 | 67.252 |
| GaN | 213.000 | | 197.682 | 198.807 | 198.521 | 198.914 | 200.704 | 201.514 | 211.373 | 182.466 |
| GaP | 89.600 | | 88.431 | 87.500 | 87.463 | 87.681 | 90.981 | 89.785 | 90.466 | 78.712 |
| GaAs | 76.700 | | 72.167 | 72.145 | 71.990 | 72.014 | 73.933 | 73.764 | 73.804 | 62.019 |
| InP | 72.000 | | 68.468 | 68.339 | 68.256 | 68.405 | 70.189 | 69.924 | 70.286 | 60.930 |
| InAs | 58.600 | | 57.540 | 57.441 | 57.289 | 57.287 | 58.911 | 58.661 | 58.929 | 49.497 |
| InSb | 46.100 | | 43.781 | 43.336 | 43.221 | 43.163 | 44.879 | 44.299 | 44.017 | 37.074 |
| LiH | 40.100 | | 37.627 | 37.545 | 37.481 | 37.453 | 40.922 | 40.751 | 36.485 | 36.343 |
| LiF | 76.300 | | 79.448 | 79.030 | 78.996 | 79.054 | 83.075 | 82.599 | 78.714 | 67.393 |
| LiCl | 38.700 | | 36.962 | 36.730 | 36.717 | 36.723 | 39.062 | 38.798 | 35.064 | 31.863 |
| NaF | 53.100 | | 60.176 | 59.892 | 59.873 | 59.867 | 60.462 | 60.157 | 59.895 | 47.016 |
| NaCl | 27.600 | | 31.288 | 31.073 | 31.063 | 31.069 | 31.723 | 31.492 | 29.140 | 24.264 |
| MgO | 169.800 | | 165.096 | 166.031 | 165.926 | 166.215 | 167.093 | 167.910 | 170.619 | 151.596 |
| Li | 13.100 | | 13.886 | 13.891 | 13.909 | 13.913 | 14.638 | 14.662 | 13.116 | 13.957 |
| Na | 7.900 | | 8.845 | 8.817 | 8.807 | 8.803 | 8.869 | 8.830 | 7.930 | 7.877 |
| K | 3.800 | | 4.144 | 4.203 | 4.196 | 4.197 | 3.956 | 3.943 | 3.422 | 3.593 |
| Rb | 3.600 | | 3.334 | 3.441 | 3.421 | 3.312 | 3.286 | 3.256 | 2.631 | 2.798 |
| Cs | 2.300 | | 2.216 | 2.197 | 2.187 | 2.181 | 2.180 | 2.151 | 1.867 | 1.960 |
| Ca | 15.900 | | 20.198 | 20.729 | 20.742 | 20.696 | 19.295 | 18.814 | 17.595 | 17.458 |
| Ba | 10.600 | | 9.514 | 9.455 | 9.440 | 9.428 | 9.444 | 9.369 | 8.569 | 8.844 |
| Sr | 12.000 | | 13.031 | 12.108 | 12.093 | 12.049 | 13.079 | 13.053 | 11.832 | 11.598 |
| Al | 77.100 | | 90.078 | 90.654 | 91.171 | 91.419 | 91.954 | 93.144 | 92.466 | 77.996 |
| Ni | 192.500 | | 226.477 | 224.995 | 223.348 | 222.570 | 229.632 | 226.624 | 216.804 | 196.258 |
| V | 165.800 | | 201.548 | 201.041 | 200.526 | 200.408 | 203.115 | 202.116 | 201.269 | 187.488 |
| Nb | 173.200 | | 179.288 | 179.820 | 179.238 | 179.021 | 180.805 | 180.736 | 178.078 | 173.453 |
| Ta | 202.700 | | 212.406 | 211.688 | 211.184 | 210.991 | 213.916 | 212.688 | 210.119 | 201.055 |
| Mo | 276.200 | | 279.506 | 278.740 | 277.833 | 277.557 | 281.413 | 279.859 | 281.995 | 268.535 |
| W | 327.500 | | 330.954 | 329.539 | 328.582 | 328.161 | 333.793 | 331.325 | 329.918 | 312.477 |
| Rh | 277.100 | | 281.216 | 279.700 | 277.697 | 276.995 | 285.003 | 281.255 | 281.584 | 258.115 |
| Ir | 362.200 | | 379.383 | 375.731 | 373.459 | 372.497 | 384.277 | 378.318 | 378.905 | 349.818 |
| Pd | 187.200 | | 194.535 | 191.866 | 189.957 | 189.064 | 198.086 | 193.530 | 186.087 | 169.148 |
| Pt | 285.500 | | 276.884 | 273.327 | 271.130 | 270.208 | 281.598 | 275.772 | 273.641 | 249.877 |
| Cu | 144.300 | | 160.228 | 155.717 | 153.997 | 152.980 | 166.597 | 160.709 | 159.969 | 138.007 |
| Ag | 105.700 | | 114.086 | 111.841 | 110.540 | 109.815 | 116.811 | 113.239 | 103.562 | 90.318 |
| Au | 182.000 | | 164.391 | 161.247 | 159.380 | 158.459 | 168.574 | 163.612 | 153.795 | 139.596 |
| ME | | | 1.856 | 0.666 | 0.223 | 0.140 | 4.375 | 2.732 | 1.367 | -9.704 |
| MAD | | | 6.740 | 6.811 | 6.602 | 6.450 | 7.200 | 6.542 | 5.963 | 11.022 |

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