Supporting Information for: "Fully-thermal meta-GGA exchange correlation free energy density functional"

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I. COMPUTATIONAL DETAILS

All simulations were run using the VASP software [1–3]. The static sc-H simulations were performed following Ref [4], with an 8-atom $2 \times 2 \times 2$ supercell and an energy cutoff of 500 eV. Static fcc-Al simulations were performed following Ref [5], using a single-atom primitive cell and an energy cutoff of 800 eV. Finally, static calculations on stishovite-type SiO_2 used an energy cutoff of 1400 eV, with the six-atom conventional cell.

AIMD simulations for warm dense H were performed following Ref. [6] and AIMD simulations on ambient water used 64 molecules in a cubic box, sampled using the Baldereschi mean-value point [7] and with an energy cutoff of 1400 eV. For the water simulations, the timestep was 1.1 fs and the simulations were run for 4900 MD steps, of which the first 980 (20%) were discarded.

II. GROUND-STATE AND TEMPERATURE-DEPENDENT ISOORBITAL INDICATOR α

The iso-orbital indicator α (α_T for fTSCAN) is a dimensionless combination of the MKS orbital kinetic energy, the Thomas-Fermi kinetic energy, and the von Weizsäcker kinetic energy. We present here the ground-state and temperature-dependent forms of these kinetic energy quantities used to compute α and α_T.

The orbital kinetic energy density is given by

$$t_{\mathrm{s}}(\{\psi_i\}) = \frac{1}{2}|\nabla\psi_i|^2. \tag{1}$$

The temperature dependence of this quantity is well-described by Mermin's extension of Kohn-Sham DFT to finite temperatures. In many electronic structure codes, this is the quantity evaluated at nonzero electronic temperatures.

$$\tau_{\mathrm{s}}^{\mathrm{MKS}}(\{\psi_i\}, T) = \frac{1}{2}\sum_{i=1}^{\infty} f_i(T)|\nabla\psi_i|^2. \tag{2}$$

with implicit temperature dependence conferred by the Fermi-Dirac occupation numbers $f_i(T)$.

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The ground-state Thomas-Fermi kinetic energy is given by

$$t_{\mathrm{TF}}(n) = 0.3 k_{\mathrm{F}}^2 n \tag{3}$$

where k_{F} is

$$k_{\mathrm{F}}(n) = (3\pi^2 n)^{1/3} \tag{4}$$

and the ground-state von Weizsäcker kinetic energy by

$$t_{\mathrm{vW}}(n, \nabla n) = \frac{|\nabla n|^2}{8n} \tag{5}$$

All together, the ground-state iso-orbital indicator α is constructed as

$$\alpha(\{\psi_i\}, n, \nabla n) = \frac{t_{\mathrm{s}} - t_{\mathrm{vW}}}{t_{\mathrm{TF}}}. \tag{6}$$

The numerator of this function is recognizable as the Pauli kinetic energy density

$$t_\theta = t_{\mathrm{s}} - t_{\mathrm{vW}}. \tag{7}$$

Under finite temperature conditions, the Pauli kinetic energy density becomes

$$\tau_\theta = \tau_{\mathrm{s}}^{\mathrm{MKS}} - t_{\mathrm{vW}}. \tag{8}$$

with $\tau_{\mathrm{s}}^{\mathrm{MKS}}$ defined in Equation 2 and t_{vW} still the ground-state Weizsäcker kinetic energy defined in Equation 5 [8].

This becomes the numerator of the temperature-dependent isoorbital indicator α_{T}, with the denominator given by the finite-temperature Thomas-Fermi kinetic energy density:

$$\tau_{\mathrm{TF}}(n, T) = t_{\mathrm{TF}}(n)\xi(t). \tag{9}$$

The temperature dependence is conferred by the multiplicative factor $\xi(t)$, which can be expressed as a combination of Fermi-Dirac integrals [9]. Here the temperature is expressed as the reduced temperature t, according to

$$t = \frac{T}{T_{\mathrm{F}}} = \frac{2}{\beta k_{\mathrm{F}}^2}. \tag{10}$$

where $\beta = (k_{\mathrm{B}} T)^{-1}$.

Then the T-dependent isoorbital indicator α_{T} can be written as:

$$\alpha_T(n, \nabla n, \{\psi_i\}) = \frac{\tau_{\mathrm{s}}^{\mathrm{MKS}}(\{\psi_i\}, T) - t_{\mathrm{vW}}(n, \nabla n)}{\tau_{\mathrm{TF}}(n, T)}. \tag{11}$$

III. SCAN AND fTSCAN EQUATIONS

We provide a complete set of equations required for the implementation of SCAN (obtained from Ref. [10]) as well as our fTSCAN functional. The temperature-dependent isoorbital indicator $\alpha_T(n, \nabla n, \{\psi\})$ is defined according to the main text as well as in Section II above.

A. Exchange: constants and parameters

Constants and parameters are identical in SCAN and fTSCAN.

$$k_0 = 0.174 \tag{12}$$

$$k_1 = 0.065 \tag{13}$$

$$a_1 = 4.9479 \tag{14}$$

$$\mu_{\mathrm{GE}} = \frac{10}{81} \tag{15}$$

$$b_2 = \sqrt{\frac{5913}{405000}} \tag{16}$$

$$b_1 = \frac{(511/13500)}{2b_2} \tag{17}$$

$$b_3 = 0.5 \tag{18}$$

$$b_4 = \frac{\mu_{\mathrm{GE}}^2}{k_1} - \frac{1606}{18225} - b_1^2 \tag{19}$$

$$c_{1\mathrm{x}} = 0.667 \tag{20}$$

$$c_{2\mathrm{x}} = 0.8 \tag{21}$$

$$d_{\mathrm{x}} = 1.24 \tag{22}$$

B. SCAN Exchange

The SCAN exchange energy is given by

$$E_{\mathrm{x}}^{\mathrm{SCAN}}[n] = \int d\mathbf{r} n(\mathbf{r}) \varepsilon_{\mathrm{x}}^{\mathrm{SCAN}}(\mathbf{r}) \tag{23}$$

where the per-particle exchange energy $\varepsilon_{\mathrm{x}}^{\mathrm{SCAN}}$ is the product of the LDA per-particle exchange energy $\varepsilon_{\mathrm{x}}^{\mathrm{LDA}}$ and the exchange enhancement factor $F_{\mathrm{x}}^{\mathrm{SCAN}}$:

$$\varepsilon_{\mathrm{x}}^{\mathrm{SCAN}}(\mathbf{r}) = \varepsilon_{\mathrm{x}}^{\mathrm{LDA}}(n) F_{\mathrm{x}}^{\mathrm{SCAN}}(s, \alpha). \tag{24}$$

The exchange enhancement factor is interpolated for values of α ranging from 0 to ∞, with $\alpha = 0$ and $\alpha \approx 1$ limits represented by h_{x}^{0} and h_{x}^{1}, respectively:

$$F_{\mathrm{x}}^{\mathrm{SCAN}}(s, \alpha) = \{h_{\mathrm{x}}^{1}(s, \alpha) + f_{\mathrm{x}}(\alpha)[h_{\mathrm{x}}^{0} - h_{\mathrm{x}}^{1}(s, \alpha)]\} g_{\mathrm{x}}(s). \tag{25}$$

The component terms h_{x}^{0}, h_{x}^{1}, and $g_{\mathrm{x}}(s)$ (as well as the interpolation function $f_{\mathrm{x}}(\alpha)$) are given by the following expressions.

$$g_{\mathrm{x}}(s) = 1 - \exp\left[\frac{-a_1}{\sqrt{s}}\right]. \tag{26}$$

$$h_{\mathrm{x}}^{0} = 1 + k_0 \tag{27}$$

$$h_{\mathrm{x}}^{1}(s, \alpha) = 1 + \frac{k_1 x(s, \alpha)}{k_1 + x(s, \alpha)} \tag{28}$$

$$x(s,\alpha) = \mu_{\mathrm{GE}} s^2 [1 + \frac{b_4 s^2}{\mu_{\mathrm{GE}}} \mathrm{exp}[-b_4 s^2/\mu_{\mathrm{GE}}]] + [b_1 s^2 + b_2(1-\alpha)\mathrm{exp}[-b_3(1-\alpha)^2]]^2 \tag{29}$$

$$f_{\mathrm{x}}(\alpha) = \begin{cases} \mathrm{exp}[\frac{-c_{1\mathrm{x}}\alpha}{(1-\alpha)}] & \alpha < 1 \\ -d_{\mathrm{x}}\mathrm{exp}[\frac{c_{2\mathrm{x}}}{(1-\alpha)}] & \alpha \geq 1 \end{cases} \tag{30}$$

C. *f*TSCAN Exchange

In fTSCAN, we obtain instead an exchange free energy with temperature dependence. The exchange enhancement factor $F_{\mathrm{x}}^{f\mathrm{TSCAN}}$ is constructed by a similar method as in SCAN, except with the use of temperature-dependent variables.

$$\mathcal{F}_{\mathrm{x}}^{f\mathrm{TSCAN}}[n,T] = \int d\mathbf{r} n(\mathbf{r}) f_{\mathrm{x}}^{f\mathrm{TSCAN}}(\mathbf{r},T) \tag{31}$$

$$f_{\mathrm{x}}^{f\mathrm{TSCAN}}(\mathbf{r},T) = f_{\mathrm{x}}^{\mathrm{KSDT}}(n,T) F_{\mathrm{x}}^{f\mathrm{TSCAN}}(s_{2\mathrm{x}},\alpha_T) \tag{32}$$

$$F_{\mathrm{x}}^{f\mathrm{TSCAN}}(s_{2\mathrm{x}},\alpha_T) = \{h_{\mathrm{x}}^1(s_{2\mathrm{x}},\alpha_T) + f_{\mathrm{x}}(\alpha_T)[h_{\mathrm{x}}^0 - h_{\mathrm{x}}^1(s_{2\mathrm{x}},\alpha_T)]\} g_{\mathrm{x}}(s) \tag{33}$$

$$g_{\mathrm{x}}(s) = 1 - \mathrm{exp}\left[\frac{-a_1}{\sqrt{s}}\right] \tag{34}$$

$$h_{\mathrm{x}}^0 = 1 + k_0 \tag{35}$$

$$h_{\mathrm{x}}^1(s_{2\mathrm{x}},\alpha_T) = 1 + \frac{k_1 x(s_{2\mathrm{x}},\alpha_T)}{k_1 + |x(s_{2\mathrm{x}},\alpha_T)|} \tag{36}$$

$$x(s_{2\mathrm{x}},\alpha_T) = \mu_{\mathrm{GE}} s_{2\mathrm{x}} [1 + \frac{b_4 s_{2\mathrm{x}}}{\mu_{\mathrm{GE}}} \mathrm{exp}[-b_4 s^2/\mu_{\mathrm{GE}}]] + [b_1 s_{2\mathrm{x}} + b_2(1-\alpha_T)\mathrm{exp}[-b_3(1-\alpha_T)^2]]^2 \tag{37}$$

$$f_{\mathrm{x}}(\alpha_T) = \begin{cases} \mathrm{exp}[\frac{-c_{1\mathrm{x}}\alpha_T}{(1-\alpha_T)}] & \alpha_T < 1 \\ -d_{\mathrm{x}}\mathrm{exp}[\frac{c_{2\mathrm{x}}}{(1-\alpha_T)}] & \alpha_T \geq 1 \end{cases} \tag{38}$$

D. Correlation: constants and parameters

Constants and parameters are identical in SCAN and fTSCAN.

$$c_{1\mathrm{c}} = 0.64 \tag{39}$$

$$c_{2c} = 1.5 \tag{40}$$

$$d_{\mathrm{c}} = 0.7 \tag{41}$$

$$b_{1\mathrm{c}} = 0.0285764 \tag{42}$$

$$b_{2\mathrm{c}} = 0.0889 \tag{43}$$

$$b_{3\mathrm{c}} = 0.125541 \tag{44}$$

$$\beta(r_{\mathrm{s}}) = 0.066725 \frac{1 + 0.1 r_{\mathrm{s}}}{1 + 0.1778 r_{\mathrm{s}}} \tag{45}$$

$$\chi_\infty = \left(\frac{3\pi^2}{16}\right)^{2/3} \frac{0.066725}{1.778(0.9 - 3[3/(16\pi)]^{2/3})} \approx 0.128025 \tag{46}$$

E. SCAN Correlation

$$E_{\mathrm{c}}^{\mathrm{SCAN}}[n] = \int d\mathbf{r} n(\mathbf{r}) \varepsilon_{\mathrm{c}}^{\mathrm{SCAN}}(\mathbf{r}) \tag{47}$$

$$\varepsilon_{\mathrm{c}}^{\mathrm{SCAN}}(\mathbf{r}) = \varepsilon_{\mathrm{c}}^{1} + f_{\mathrm{c}}(\alpha)(\varepsilon_{\mathrm{c}}^{0} - \varepsilon_{\mathrm{c}}^{1}) \tag{48}$$

$$\varepsilon_{\mathrm{c}}^{1} = \varepsilon_{\mathrm{c}}^{\mathrm{LDA}} + H_{\mathrm{c}}^{1} \tag{49}$$

$$H_{\mathrm{c}}^{1} = \gamma \ln[1 + w_1(1 - g(Aq^2))] \tag{50}$$

$$w_1 = \exp\left[-\frac{\varepsilon_{\mathrm{c}}^{\mathrm{LDA}}}{\gamma}\right] - 1 \tag{51}$$

$$g(Aq^2) = \frac{1}{(1 + 4Aq^2)^{1/4}} \tag{52}$$

$$A = \frac{\beta(r_{\mathrm{s}})}{\gamma w_1} \tag{53}$$

$$\varepsilon_{\mathrm{c}}^{0} = \varepsilon_{\mathrm{c}}^{\mathrm{LDA0}} + H_{\mathrm{c}}^{0} \tag{54}$$

$$\varepsilon_{\mathrm{c}}^{\mathrm{LDA0}} = -\frac{b_{1\mathrm{c}}}{1 + b_{2\mathrm{c}}\sqrt{r_{\mathrm{s}}} + b_{3\mathrm{c}} r_{\mathrm{s}}} \tag{55}$$

$$H_{\mathrm{c}}^{0} = b_{1\mathrm{c}} \ln\left[1 + w_0(1 - g_\infty)\right] \tag{56}$$

$$w_0 = \exp\left[-\frac{\varepsilon_{\mathrm{c}}^{\mathrm{LDA0}}}{b_{1\mathrm{c}}}\right] - 1 \tag{57}$$

$$g_\infty(s) = \frac{1}{(1 + 4\chi_\infty s^2)^{1/4}} \tag{58}$$

$$f_{\mathrm{c}}(\alpha) = \begin{cases} \exp[\frac{-c_{1\mathrm{c}}\alpha}{(1-\alpha)}] & \alpha < 1 \\ -d_{\mathrm{c}}\exp[\frac{c_{2\mathrm{c}}}{(1-\alpha)}] & \alpha \geq 1 \end{cases} \tag{59}$$

F. *f*TSCAN Correlation

$$\mathcal{F}_{\mathrm{c}}^{f\mathrm{TSCAN}}[n, T] = \int d\mathbf{r} n(\mathbf{r}) f_{\mathrm{c}}^{f\mathrm{TSCAN}}(\mathbf{r}, T) \tag{60}$$

$$f_{\mathrm{c}}^{f\mathrm{TSCAN}}(\mathbf{r}, T) = f_{\mathrm{c}}^{1} + f_{\mathrm{c}}(\alpha_T)(f_{\mathrm{c}}^{0} - f_{\mathrm{c}}^{1}) \tag{61}$$

$$f_{\mathrm{c}}^{1} = f_{\mathrm{c}}^{\mathrm{KSDT}} + H_{\mathrm{c}}^{1} \tag{62}$$

$$H_{\mathrm{c}}^{1} = \gamma \ln[1 + w_1(1 - g(Aq_{\mathrm{c}}^2))] \tag{63}$$

$$w_1 = \exp\left[-\frac{f_{\mathrm{c}}^{\mathrm{KSDT}}}{\gamma}\right] - 1 \tag{64}$$

$$g(Aq_{\mathrm{c}}^2) = \frac{1}{(1 + 4Aq_{\mathrm{c}}^2)^{1/4}} \tag{65}$$

$$A = \frac{\beta(r_{\mathrm{s}})}{\gamma w_1} \tag{66}$$

$$f_{\mathrm{c}}^{0} = \varepsilon_{\mathrm{c}}^{\mathrm{LDA0}} \lambda(t) + H_{\mathrm{c}}^{0} \tag{67}$$

$$\varepsilon_{\mathrm{c}}^{\mathrm{LDA0}} = -\frac{b_{1\mathrm{c}}}{1 + b_{2\mathrm{c}}\sqrt{r_{\mathrm{s}}} + b_{3\mathrm{c}} r_{\mathrm{s}}} \tag{68}$$

$$\lambda(t) = \frac{f_{\mathrm{c}}^{\mathrm{KSDT}}(n, T)}{f_{\mathrm{c}}^{\mathrm{KSDT}}(n, T = 1^{-10})} \tag{69}$$

$$H_{\mathrm{c}}^{0} = b_{1\mathrm{c}} \ln\left[1 + w_0(1 - g_{\infty}(q_{\mathrm{c}}))\right] \tag{70}$$

$$w_0 = \exp\left[-\frac{\varepsilon_{\mathrm{c}}^{\mathrm{LDA0}} \lambda(t)}{b_{1\mathrm{c}}}\right] - 1 \tag{71}$$

$$g_{\infty}(q_{\mathrm{c}}) = \frac{1}{(1 + 4\chi_{\infty} q_{\mathrm{c}}^2)^{1/4}} \tag{72}$$

$$f_{\mathrm{c}}(\alpha_T) = \begin{cases} \exp[\frac{-c_{1\mathrm{c}}\alpha_T}{(1-\alpha_T)}] & \alpha_T < 1 \\ -d_{\mathrm{c}}\exp[\frac{c_{2\mathrm{c}}}{(1-\alpha_T)}] & \alpha_T \geq 1 \end{cases} \tag{73}$$

G. Additional details for $\lambda(r_\mathrm{s}, t)$ multiplicative thermalization factor

The T-dependent scaling factor $\lambda(r_\mathrm{s}, t)$ is used to add temperature dependence to the reference $\varepsilon_\mathrm{c}^\mathrm{LDA0}$ energy (Eq. 68), as seen in Eq. 67. This factor is obtained from a pair of calculations using the T-dependent LDA-level KSDT XC functional [11], one at the temperature of interest and the other at low-T ($t = 10^{-4}$). $\lambda(r_\mathrm{s}, t)$ is then constructed as defined in Eq. 69:

$$\lambda(t) = \frac{f_\mathrm{c}^\mathrm{KSDT}(n, T)}{f_\mathrm{c}^\mathrm{KSDT}(n, T = 1^{-10})} \tag{69}$$

Figure 1 shows $\lambda(r_\mathrm{s}, t)$ for $r_\mathrm{s} = 0.5$ and $r_\mathrm{s} = 4$. $\lambda(r_\mathrm{s}, t)$ smoothly reduces to 1 as $t \to 0$, recovering the ground state, has a maximum around $t = 1$, and finally vanishes at large t.

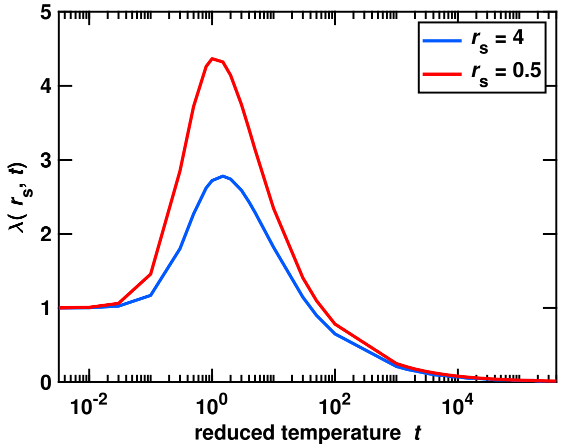

FIG. 1. Thermal multiplicative factor $\lambda(r_\mathrm{s}, t)$ computed for $r_\mathrm{s} = 0.5$ (red) and $r_\mathrm{s} = 4$ (blue).

H. Tabulated data for static calculations

TABLE I. Electronic pressures for *sc*-H at a range of electronic pressures calculated using PBE, KDT16, SCAN, and fTSCAN functionals.

T (eV)	P^{PBE} (Mbar)	P^{KDT16} (Mbar)	P^{SCAN} (Mbar)	$P^{f\mathrm{TSCAN}}$ (Mbar)
0.0861735	116.985	122.177	102.014	106.526
0.1292602	117.266	122.522	102.208	106.709
0.1723469	117.933	123.281	102.794	107.291
0.2585204	120.214	125.821	104.895	109.389
0.3446939	123.626	129.585	108.078	112.584
0.4308673	128.108	134.503	112.274	116.805
0.5170408	133.616	140.520	117.451	122.007
0.6893877	147.520	155.612	130.560	135.144
0.86173467	164.982	174.395	147.103	151.563
1.29260201	222.437	235.114	201.660	204.145
1.72346934	297.278	311.956	272.869	268.921
2.58520402	490.081	496.680	456.501	420.610
3.44693869	727.611	704.496	683.172	599.827
4.30867336	998.770	932.644	942.983	816.000
5.17040803	1296.749	1184.474	1230.606	1071.942
6.0321427	1617.239	1461.853	1542.208	1363.943
6.89387738	1957.046	1763.939	1875.593	1686.389
7.75561205	2313.586	2088.620	2228.095	2033.055
8.61734672	2684.573	2432.908	2595.661	2398.642
10.7716834	3663.850	3361.655	3574.543	3370.611
12.9260201	4699.780	4366.360	4619.976	4400.859
15.0803568	5777.014	5434.436	5718.233	5480.322
17.2346934	6884.960	6555.388	6853.611	6604.287
21.5433668	9166.119	8902.020	9192.058	8942.793
25.8520402	11506.076	11320.602	11572.660	11344.372
30.1607135	13884.394	13770.775	13985.936	13777.456
34.4693869	16288.240	16235.630	16419.662	16230.562

TABLE II. Electronic pressures for fcc-Al at a range of electronic pressures calculated using PBE, KDT16, SCAN, and *f*TSCAN functionals.

T (eV)	P^{PBE} (Mbar)	P^{KDT16} (Mbar)	P^{SCAN} (Mbar)	$P^{f\mathrm{TSCAN}}$ (Mbar)
0.0861735	96.54	100.16	70.49	74.12
0.1292602	97.10	100.77	71.25	74.98
0.1723469	97.89	101.60	72.16	76.02
0.2585204	99.98	103.83	74.45	78.68
0.3446939	102.62	106.66	77.31	82.04
0.4308673	105.82	110.08	80.74	86.04
0.5170408	109.62	114.15	84.78	90.72
0.6893877	119.02	124.10	95.05	102.19
0.86173467	131.10	136.66	108.7	116.61
1.29260201	172.86	178.37	158.12	163.71
1.72346934	230.27	232.75	214.56	218.98
2.58520402	381.16	365.58	353.86	346.18
3.44693869	565.51	522.61	504.12	498.64
4.30867336	771.08	699.23	677.23	674.66
5.17040803	989.19	889.85	888.96	868.41
6.0321427	1214.40	1090.65	1128.46	1074.06
6.89387738	1443.86	1298.94	1376.30	1288.24
7.75561205	1675.46	1512.07	1622.64	1506.86
8.61734672	1908.69	1728.85	1865.85	1728.37
9.47908139	2142.70	1948.45	2108.36	1952.30
10.3408161	2377.22	2170.82	2351.59	2178.27
12.0642854	2847.09	2624.64	2841.16	2636.49
13.7877547	3317.37	3088.70	3329.39	3103.40
15.51122409	3787.66	3559.82	3812.88	3575.77
17.23469344	4258.24	4035.63	4290.21	4051.18
18.95816278	4729.56	4514.70	4764.02	4528.11
20.68163213	5202.08	4996.15	5239.88	5004.65
22.40510147	5676.22	5479.44	5715.50	5480.65
24.12857081	6151.77	5964.86	6192.94	5961.56

TABLE III. Electronic pressures for stishovite SiO_2 for selected unit cell volumes calculated using LDA (PZ), PBE, PBEsol, KDT16, SCAN, and fTSCAN functionals. All pressures are in units of GPa.

V (Å/F.U.)	P^{LDA} (GPa)	P^{PBE}	P^{PBEsol}	P^{KDT16}	P^{SCAN}	$P^{f\mathrm{TSCAN}}$
20.685	40.93	56.77	49.59	58.22	47.87	49.73
20.895	36.06	51.68	44.61	53.11	42.75	44.58
21.115	31.20	46.57	39.64	47.97	37.62	39.42
21.350	26.31	41.45	34.63	42.81	32.46	34.22
21.600	21.46	36.35	29.65	37.69	27.33	29.06
21.865	16.58	31.22	24.65	32.53	22.18	23.85
22.145	11.73	26.11	19.66	27.38	17.05	18.66
22.450	6.89	20.99	14.67	22.23	11.92	13.47
22.775	2.07	15.89	9.71	17.10	6.81	8.30
22.915	0.14	13.84	7.71	15.03	4.76	6.23

[1] G. Kresse and J. Furthmüller, Efficient iterative schemes for *ab initio* total-energy calculations using a plane-wave basis set, Phys. Rev. B **54**, 11169 (1996).

[2] G. Kresse and J. Furthmüller, Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set, Comput. Mater. Sci. **6**, 15 (1996).

[3] G. Kresse and D. Joubert, From ultrasoft pseudopotentials to the projector augmented-wave method, Phys. Rev. B **59**, 1758 (1999).

[4] V. V. Karasiev, D. I. Mihaylov, and S. X. Hu, Meta-GGA exchange-correlation free energy density functional to increase the accuracy of warm dense matter simulations, Phys. Rev. B **105**, L081109 (2022).

[5] V. V. Karasiev, J. W. Dufty, and S. B. Trickey, Nonempirical Semilocal Free-Energy Density Functional for Matter under Extreme Conditions, Phys. Rev. Lett. **120**, 076401 (2018).

[6] M. Bonitz, J. Vorberger, M. Bethkenhagen, M. Böhme, D. Ceperley, A. Filinov, T. Gawne, F. Graziani, G. Gregori, P. Hamann, S. Hansen, M. Holzmann, S. X. Hu, H. Kählert, V. Karasiev, U. Kleinschmidt, L. Kordts, C. Makait, B. Militzer, Z. Moldabekov, C. Pierleoni, M. Preising, K. Ramakrishna, R. Redmer, S. Schwalbe, P. Svensson, and T. Dornheim, Towards first principles-based simulations of dense hydrogen, Phys. Plasmas **31**, 110501 (2024).

[7] A. Baldereschi, Mean-Value Point in the Brillouin Zone, Phys. Rev. B **7**, 5212 (1973).

[8] R. M. N. Goshadze, V. V. Karasiev, K. P. Hilleke, and S. X. Hu, On the Pauli Potential Formalism at Finite Temperature, In preparation (2024).

[9] V. V. Karasiev, T. Sjostrom, and S. B. Trickey, Generalized-gradient-approximation noninteracting free-energy functionals for orbital-free density functional calculations, Phys. Rev. B **86**, 115101 (2012).

[10] J. Sun, A. Ruzsinszky, and J. P. Perdew, Strongly Constrained and Appropriately Normed Semilocal Density Functional, Phys. Rev. Lett. **115**, 036402 (2015).

[11] V. V. Karasiev, T. Sjostrom, J. Dufty, and S. B. Trickey, Accurate Homogeneous Electron Gas Exchange-Correlation Free Energy for Local Spin-Density Calculations, Phys. Rev. Lett. **112**, 076403 (2014).