

Erratum: Influence of finite temperature exchange-correlation effects in hydrogen [Phys. Rev. B **101**, 195129 (2020)]

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We have identified a computational error in our simulations requiring correction. The main conclusions of our study remain unaffected, and the correction involves properly evaluating the thermal exchange-correlation contributions at the temperature considered in our simulations.

Simulation details. Following the publication of our original article, we discovered that the thermal exchange-correlation (XC) contributions had been evaluated at an incorrect temperature due to a bug in the library of exchange-correlation functionals (LIBXC) [1]. Moreover, we note that at low densities, the evaluation of the equation of state (EOS) using a plane-wave basis [2–6] shows significant deviations at temperatures greater than 40 000 K compared to the localized basis set [7,8].

In a recent collaborative effort on first-principles simulations of dense hydrogen [9], some of the issues arising from our original article were discussed, and henceforth we address the issues in this Erratum. The new set of calculations is performed using the Vienna *ab initio* simulation package (VASP) [2–5]. The finite temperature XC functional (GDSMFB) [10] is accessed using LIBXC. The simulations utilize the projector augmented-wave (PAW) pseudopotential (PAW_H_06May1998). Brillouin-zone sampling is carried out at the Baldereschi mean value point [11]. A 600 eV plane-wave cutoff is applied and the convergence criterion is set for each self-consistency to 10^{-5} . We employ the Mermin thermal density functional theory (DFT) formulation, which incorporates Fermi-Dirac occupations for electronic states [12]. Simulations are carried out in the NVT ensemble, controlled by a Nose-Hoover thermostat [13]. In this Erratum, the XC potential is derived using $v_{xc} = \frac{\partial(nf_{xc})}{\partial n}$ similar to the work described by Karasiev *et al.* [14] where f_{xc} is the parametrized form of the XC free energy per particle parametrized by Groth *et al.* [10].

Results. Figure 1 shows the EOS calculated at $r_s = 2, 3, 4, 5, 10$, and 14 comparing our current results evaluated using GDSMFB [10,15] and Perdew-Zunger (PZ) [16] XC functionals, previous results [9], path integral Monte Carlo (PIMC) [17,18], and DFT [9] simulations. Figure 2 shows the relative difference in pressure for the finite temperature case (GDSMFB) with respect to the local density approximation (LDA) (PZ) using

$$\Delta P = \left(\frac{P_{PZ} - P_{GDSMFB}}{P_{PZ}} \right) \times 100 \quad (1)$$

based on the data shown in Fig. 1.

Figures 3 and 4 show the relative difference in pressure for finite temperature LDA (GDSMFB) relative to ground state LDA (PZ) with respect to the Wigner-Seitz radius (r_s) and the electron degeneracy ($\theta = T/T_F$) at $T = 62\,500$ K and $T = 31\,250$ K, respectively. In comparison, the relative difference in pressure for the finite temperature generalized gradient approximation (GGA) functional KDT16 [19] with respect to Perdew-Burke-Ernzerhof (PBE) [20] calculated using

$$\Delta P = \left(\frac{P_{PBE} - P_{KDT16}}{P_{PBE}} \right) \times 100 \quad (2)$$

is also shown [9].

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Data availability. No data were created or analyzed in this study.

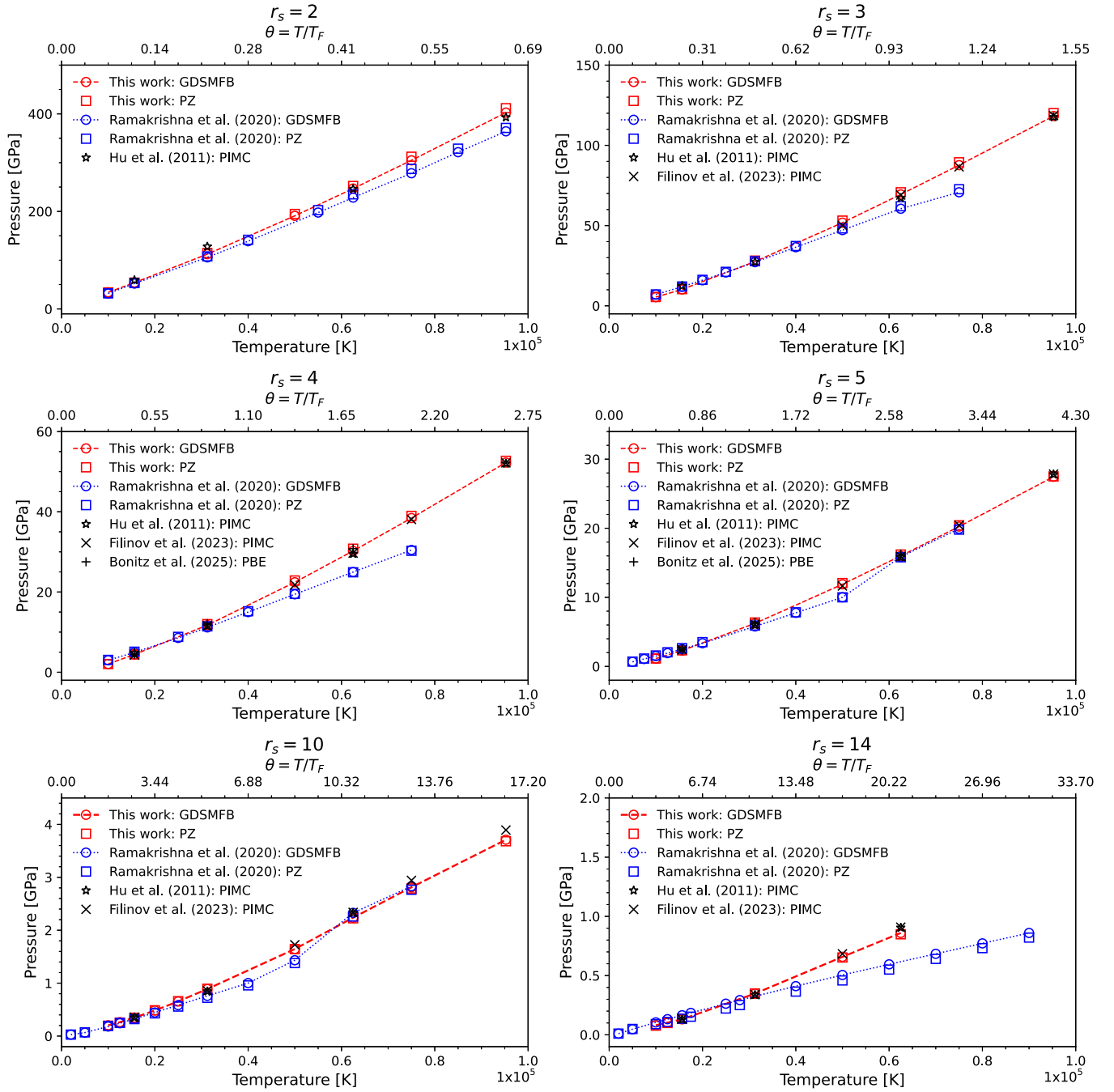


FIG. 1. Equation of state at $r_s = 2, 3, 4, 5, 10$, and 14 comparing our results (GDSMFB [10] and PZ [16]) with the previous results obtained using PIMC [17,18] and DFT [9].

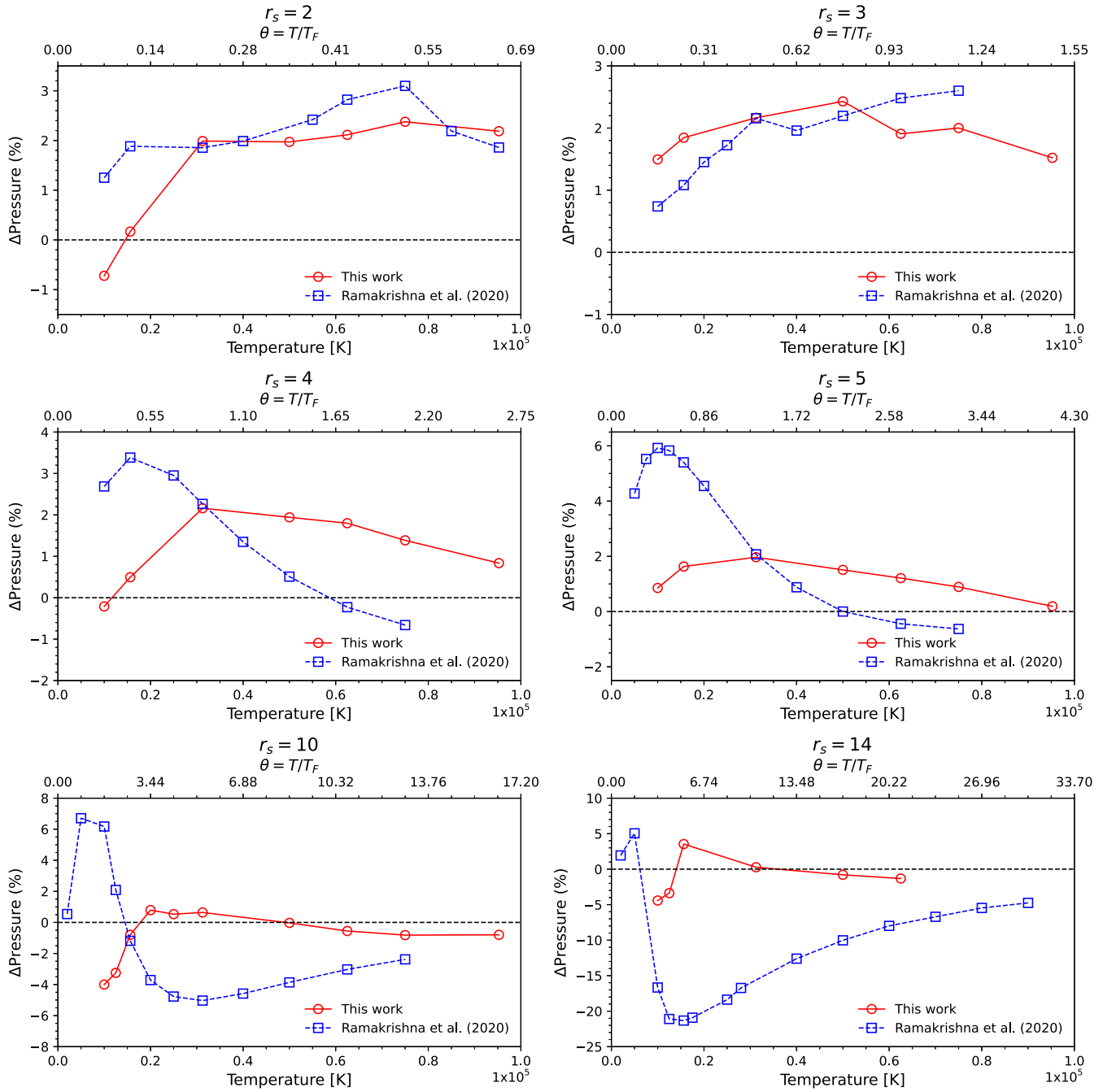


FIG. 2. Relative difference in pressure for the finite temperature case (GDMSFB) with respect to LDA (PZ) computed using $\Delta P(\%) = (P_{PZ} - P_{GDMSFB})/P_{PZ}$ based on the data presented in Fig. 1.

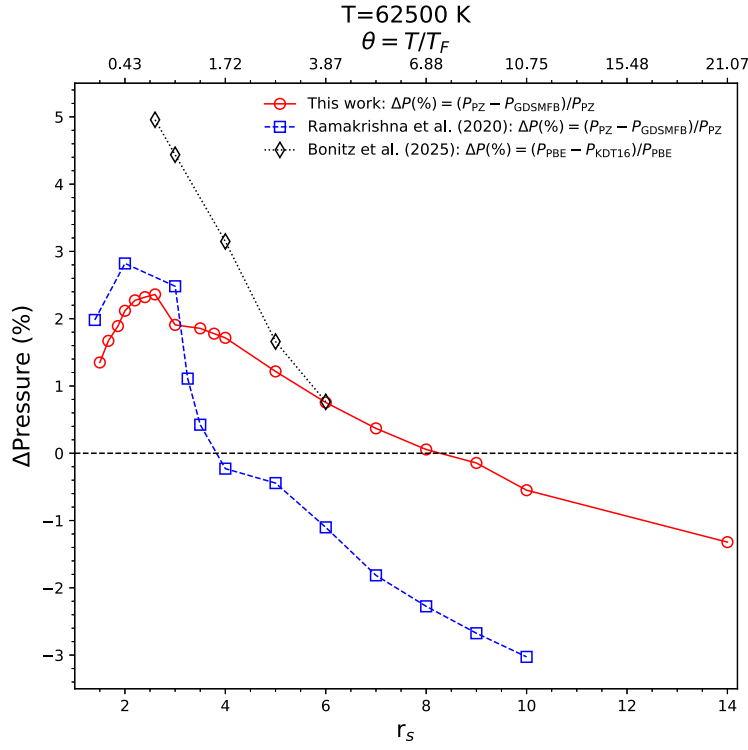


FIG. 3. Relative difference in pressure for the finite temperature case (GDSMFB) with respect to LDA (PZ) computed using $\Delta P(\%) = (P_{\text{PZ}} - P_{\text{GDSMFB}})/P_{\text{PZ}}$ with respect to the Wigner-Seitz radius (r_s) and electron degeneracy ($\theta = T/T_F$) at $T = 62\,500$ K. In comparison, the relative difference in pressure for the finite temperature GGA (KDT16) [19] with respect to PBE [20] computed using $\Delta P(\%) = (P_{\text{PBE}} - P_{\text{KDT16}})/P_{\text{PBE}}$ is also shown [9].

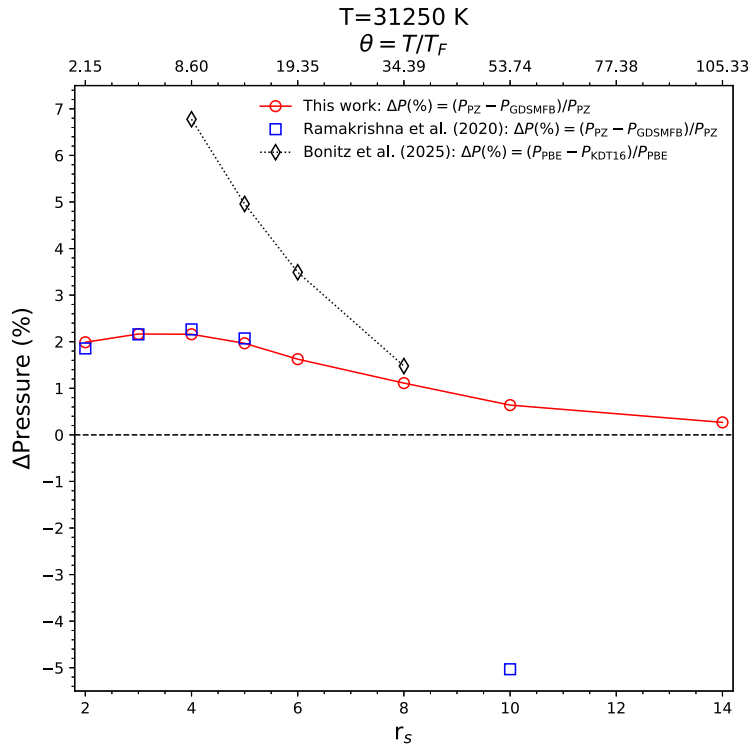


FIG. 4. Relative difference in pressure for the finite temperature case (GDSMFB) with respect to LDA (PZ) computed using $\Delta P(\%) = (P_{\text{PZ}} - P_{\text{GDSMFB}})/P_{\text{PZ}}$ with respect to the Wigner-Seitz radius (r_s) and electron degeneracy ($\theta = T/T_F$) at $T = 31\,250$ K. In comparison, the relative difference in pressure for the finite temperature GGA (KDT16) [19] with respect to PBE [20] computed using $\Delta P(\%) = (P_{\text{PBE}} - P_{\text{KDT16}})/P_{\text{PBE}}$ is also shown [9].

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