

Erratum: Orbital-free kinetic-energy functionals for the nearly free electron gas [Phys. Rev. B 58, 13465 (1998)]

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(Published 5 September 2001)

DOI: 10.1103/PhysRevB.64.129901

PACS number(s): 71.15.Mb, 99.10.+g

In the published version of the erratum,¹ the values in Table III were misprinted. Below is the correct version of the erratum in its entirety.

After the publication of our previous paper,² we found that the real-space evaluation of $\nabla\rho(\mathbf{r})$ (needed for the evaluation of $T_{vw}[\rho]$) was strongly affected by the fineness of the mesh chosen for a given simulation cell, the plane-wave cutoff (400 eV) used for the Goodwin-Needs-Heine local pseudopotential for aluminum³ was not sufficient, and the Kohn-Sham (KS) calculations (used for comparison with the HK orbital-free calculations) had not been fully converged with respect to the \mathbf{k} -point sampling.⁴ To remedy the first problem, we now evaluate $\nabla\rho(\mathbf{r})$ in momentum space.⁵ This scheme is very stable (up to 0.001 eV) against changes of the mesh beyond a certain minimum mesh size. We also increased the plane-wave cutoff to 600 eV, and converged the KS calculations with respect to the \mathbf{k} -point sampling.⁴ The KS calculations were performed using the plane-wave density-functional theory (DFT) code CASTEP,⁶ with the finest \mathbf{k} -point sampling allowed by the code. The exchange-correlation effects were treated at the local-density approximation level.⁷ The corrected Tables II and III summarize the final results for different bulk phases of aluminum, which should serve as corrections to our previous paper.² We do not

include the information for the expansion weights $\{\lambda_\alpha\}$ since they are readily available from Table I in Ref. 2.

For the sake of completeness, we also calculated the vacancy formation (vf) energy⁸ using a 4-site cell (3 atoms + 1 vacancy). Since our plane-wave cutoff and \mathbf{k} -point sampling are converged further than previous reports,⁹ we use our KS vf numbers as the benchmark.

After comparing the tables, we find some sizable differences between our previous values² and new results, especially for the vf energies. The “good” agreement is no longer there. Moreover, in terms of absolute energies, $T_s^{1/2}$ is the worst among all these kinetic-energy density functionals (KEDF’s) in Tables II and III; $T_s^{5/6}$ does quite well by comparison. This is not surprising because $T_s^{1/2}$ only takes care of the $q \rightarrow 0$ limit, but does a poor job describing the $q \rightarrow \infty$ limit. As we pointed out before,² the fulfillment of the $q \rightarrow \infty$ limit is much more important than that of the $q \rightarrow 0$ limit. For the same reason, other KEDF’s shown here perform better. However, the more general KEDF’s made from a

TABLE III. Calculated energy per atom (eV) for bulk aluminum. The last two columns are the vacancy formation (vf) energies, and the first column is the energy for the fcc structure, while other columns are energy increments from the fcc structure. “sc” stands for simple cubic and “dia” for diamond.

Model ^a	fcc	hcp ^b	bcc	sc	dia	vf4 ^c	vf32 ^c
Kohn-Sham	-58.336	0.060	0.068	0.250	0.599	0.646	0.626
{1}	-58.300	0.040	0.049	0.232	0.521	1.135	1.562
$\{\frac{5}{6}\}$	-58.331	0.050	0.060	0.227	0.673	1.104	1.371
$\{\frac{1}{2}\}$	-58.440	0.079	0.099	0.175	0.595	0.748	0.482
$\{\sqrt{5}/3\}$	-58.351	0.055	0.068	0.220	0.703	1.065	1.230
$\{\frac{5}{6}, \frac{1}{2}\}$	-58.343	0.053	0.065	0.222	0.679	1.076	1.280
{0.511,0.402}	-58.390	0.066	0.082	0.204	0.716	0.979	0.975
$\{\frac{5}{6}, \frac{1}{2}, 1\}$	-58.411	0.074	0.092	0.209	0.863	1.020	0.959
$\{\frac{5}{6}, \frac{1}{2}, \frac{2}{3}\}$	-58.401	0.070	0.087	0.204	0.771	0.986	0.953

^aThe exponents $\{\alpha\}$ are shown here for $T_s^{(\alpha)}$; their corresponding expansion weights $\{\lambda_\alpha\}$ are available from Table I in Ref. 2.

^bThe hcp calculations were performed using the fcc nearest neighbor distance for each case.

^cvf4 is for 4-site simulation cell (3 atoms + 1 vacancy); vf32 is for 32-site simulation cell (31 atoms + 1 vacancy). The experimental vf number is 0.66 eV (Ref. 9).

TABLE II. Calculated lattice parameters (Å) for bulk aluminum. “sc” stands for simple cubic and “dia” for diamond. Lattice parameters refer to cell size in the cubic unit cell: fcc cell, 4 atoms; bcc cell, 2 atoms; sc cell, 8 atoms; and dia cell, 8 atoms.

Model ^a	fcc	bcc	sc	dia
Kohn-Sham	4.03	3.23	5.33	5.84
{1}	4.06	3.25	5.34	6.05
$\{\frac{5}{6}\}$	4.04	3.23	5.33	5.94
$\{\frac{1}{2}\}$	3.96	3.17	5.31	5.95
$\{\sqrt{5}/3\}$	4.03	3.22	5.32	5.92
$\{\frac{5}{6}, \frac{1}{2}\}$	4.03	3.22	5.32	5.94
{0.511,0.402}	4.00	3.20	5.31	5.89
$\{\frac{5}{6}, \frac{1}{2}, 1\}$	3.99	3.19	5.30	5.81
$\{\frac{5}{6}, \frac{1}{2}, \frac{2}{3}\}$	4.00	3.20	5.30	5.86

^aThe exponents $\{\alpha\}$ are shown here for $T_s^{(\alpha)}$; their corresponding expansion weights $\{\lambda_\alpha\}$ are available from Table I in Ref. 2.

combination of several single KEDF's as in Eq. (26) of Ref. 2 do not enhance the performance as much as we previously thought. We also tried other KEDF's of different combinations according to the scheme presented earlier,² but the re-

sults did not improve much. This indicates that fulfillment of the $q \rightarrow \infty$ limit and elimination of those spurious $\delta\sigma$ terms must be taken into consideration concurrently, while the $q \rightarrow 0$ limit is of secondary importance.

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