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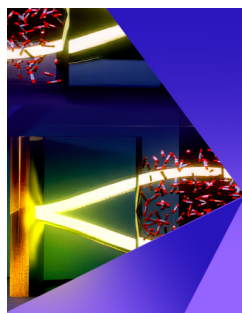
## Erratum: "Assessment of interaction-strength interpolation formulas for gold and silver clusters" [J. Chem. Phys. 148, 134106 (2018)] ✓

Sara Giarrusso; Paola Gori-Giorgi; Fabio Della Sala ; Eduardo Fabiano 



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## Erratum: “Assessment of interaction-strength interpolation formulas for gold and silver clusters” [J. Chem. Phys. **148**, 134106 (2018)]

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With this Erratum, we provide corrections to certain mistakes appearing in the original publication.<sup>1</sup>

Namely, in Eq. (12), the  $\lambda$ -dependent Hamiltonian for the Hartree-Fock adiabatic connection lacks the external potential term. The correct equation is

$$\hat{H}^\lambda = \hat{T} + \hat{V}_{\text{HF}} + \hat{V}_{\text{ext}} + \lambda(\hat{V}_{ee} - \hat{V}_{\text{HF}}). \quad (1)$$

The typos listed in the following all appear in the appendix. The parameter  $c$  in Eq. (A6) is wrong by a factor of two; the correct expression reads as follows:

$$c = \frac{4(W'_0 W'_\infty)^2}{(W_0 - W_\infty)^4}. \quad (2)$$

In Eq. (A13), we have incorrectly used the parameter “ $c$ ”; “ $c$ ” has to be replaced by “ $\gamma$ ,” as defined in Eq. (A12). Also, the expression lacks the exchange energy. Thus, the proper expression reads as follows:

$$E_{xc}^{\text{LB}} = 2\beta \left[ \frac{1}{\gamma} \left( \sqrt{1 + \gamma} - \frac{1 + \gamma/2}{1 + \gamma} \right) - 1 \right] + W_0. \quad (3)$$

Finally, in Eqs. (A14) and (A15), the fractional powers appearing in the first terms are powers of the density and not of the position vector. Hence,

$$W_\infty \approx W_\infty^{\text{PC}} = \int \left[ A \rho^{4/3}(\mathbf{r}) + B \frac{|\nabla \rho(\mathbf{r})|^2}{\rho^{4/3}(\mathbf{r})} \right] d\mathbf{r}, \quad (4)$$

$$W'_\infty \approx W'_\infty^{\text{PC}} = \int \left[ C \rho^{3/2}(\mathbf{r}) + D \frac{|\nabla \rho(\mathbf{r})|^2}{\rho^{7/6}(\mathbf{r})} \right] d\mathbf{r}. \quad (5)$$

These corrections do not alter any of the results or conclusions shown in the paper.

<sup>1</sup>S. Giarrusso, P. Gori-Giorgi, F. Della Sala, and E. Fabiano, *J. Chem. Phys.* **148**, 134106 (2018).