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ERRATUM

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Fully Numerical All-Electron Solutions of the Optimized Effective Potential Equation for Diatomic Molecules [*Journal of Chemical Theory and Computation* **2009**, *5*, 1731–1740. DOI: 10.1021/ct800485v]. Adi Makmal, Stephan Kümmel, and Leeor Kronik*

With this Erratum, we provide corrections for minor technical errors we found in our original publication.[1] These corrections do not alter any of the conclusions drawn in the paper:

(1) In Table 9, the xOEP 1σ eigenvalue of LiH should be $-2.06(6)$ Hartree.

(2) In appendix B, eq (B4) should be

$$\varepsilon^1_{i\sigma} = \langle\varphi_{i\sigma}|\Delta v_{i\sigma}|\varphi_{i\sigma}\rangle + \langle\psi_{i\sigma}|H_{KS}|\varphi_{i\sigma}\rangle^* - \langle\varphi_{i\sigma}|H_{KS}|\psi_{i\sigma}\rangle$$

where the Kohn−Sham eigenvalues are assumed to be real. This differs from the form given in the original article by complex conjugation of the second term on the right-hand side of the equation and by the sign of the third term on the right-hand side of the equation.

(3) In appendix B, eq (B5) should be

$$\underbrace{\left[H_{KS} - \varepsilon^0_{i\sigma} + \varepsilon^0_{i\sigma}|\varphi_{i\sigma}\rangle\langle\varphi_{i\sigma}| - |\varphi_{i\sigma}\rangle\langle\varphi_{i\sigma}|H_{KS}\right]}_{A} \underbrace{|\psi_{i\sigma}\rangle}_{x} =$$

$$\underbrace{-(\overline{\Delta v}_{i\sigma}(\mathbf{r}) - \Delta v_{i\sigma}(\mathbf{r}))|\varphi_{i\sigma}\rangle}_{b}$$

This differs from the form given in the original article by sign of the third term on the left-hand side of the equation.

(4) Our mention of previous optimized effective potential work for single atoms unfortunately omitted the work of Cinal and Holas.[2]

REFERENCES

(1) Makmal, A.; Kümmel, S.; Kronik, L. *J. Chem. Theory Comput.* **2009**, *5*, 1731.

(2) Cinal, M.; Holas, A. *Phys. Rev. A* **2007**, *76*, 042510.

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