

This Week's Citation Classic®

Perdew J P & Zunger A. Self-interaction correction to density-functional approximations for many-electron systems. *Phys. Rev. B—Condensed Matter* 23:5048-79, 1981. [Tulane University, New Orleans. LA and Solar Energy Research Institute, Golden. CO]

In the local-spin-density approximation, each electron interacts weakly with itself. By subtracting out the spurious self-interaction on an orbital-by-orbital basis, we found improved values for the exchange, correlation, and total energies of atoms, as well as orbital eigenvalues that closely approximated physical removal energies in atoms and solids. The self-interaction correction for fractional electron number led to the later discovery of the derivative discontinuity of the exact energy. [The *SC²* indicates that this paper has been cited in more than 1,125 publications.]

Freshman Physics in Many-Body Theory

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Today's journals abound with density-functional calculations for the structure and energetics of atoms, molecules, and solids. This theory¹ reduces the ground-state many-electron problem to self-consistent one-electron form. Back in 1978, as a new assistant professor at Tulane, I was bothered by the fact that the local-spin-density approximation¹ is not exact for one-electron problems like the hydrogen atom. In the course of getting the difficult many-body physics almost right, this approximation was flunking freshman physics by making an electron interact with itself. By subtracting out the spurious self-interaction on an orbital-by-orbital basis, I got a better description of the exchange energy, the correlation energy, the highest-occupied orbital energy, etc.

This idea, motivated by a simple limit and already applied to the exchange potential by Lindgren, came after my six happy years as a postdoctoral fellow, exploring the local approximation and possible improvements thereof with Sy Vosko and Dave Langreth. Only later did I discover a long history of attempts at self-interaction correction. After a ten-minute talk about my results at the 1979 March meeting of the American Physical Society, Alex Zunger stood

up and said that he and Art Freeman had done something similar, correcting about 90 percent of the local-density error in the core and valence excitation spectra of solid lithium fluoride via a self-interaction-corrected supercell calculation.²

Alex and I began a collaboration in which he did nearly all the applications, and I did most of the formalism. Writing this long paper was a chore, and at times a tug-of-war. Because he was the first author of the letter version, I was first on the big paper—only for this reason do most citations appear to accrue to me.

After our "SIC" (self-interaction correction) paper was published, I began to hear "SIC" jokes. Because our potential was orbital-dependent, unlike the Kohn-Sham potential, our work was scorned by a few density-functional purists. Although counting ourselves in that synod, we chose freshman physics over orthodoxy.

Our paper is cited for various reasons: (1) The self-interaction correction turned out to improve the results of the local approximation, not only for atoms but also for negative ions, insulators, high-temperature superconductors, and the Hubbard model.^{3,4} The magnetic moments and band gaps of the transition-metal oxides were greatly improved.⁵ (2) Its extension from atoms to molecules and solids proved to be a subtle and challenging problem.^{3,5} (3) Our paper was so massive that it served as a review of density functional theory, now supplanted by excellent books⁶ and review articles. (4) The self-interaction correction for fractional particle number suggested the later discovery of derivative discontinuities³ of the exact energy, with implications for the highest-occupied orbital energy and for the fundamental band gap of an insulator. But the most common reason is the least honorific one: (5) In an appendix, I presented a continuation to higher densities of the Ceperley-Alder correlation energy for a uniform electron gas, which is still widely used in density functional calculations. Today, these calculations are usually of the local-spin-density or gradient-corrected type, without self-interaction correction.

Recently I have discovered a new use for the *Science Citation Index*[®], to evaluate the panels that award millions of taxpayer dollars for research.

1. Kohn W & Sham L J. Self-consistent equations including exchange and correlation effects. *Phys. Rev.* 140:A1133-40, 1965. (Cited 3,630 times.)

2. Zunger A & Freeman A J. Ground- and excited-state properties of LiF in the local-density formalism. *Phys. Rev. B—Solid State* 16:2901-26, 1977. (Cited 110 times.)

3. Perdew J P. Size-consistency, self-interaction correction, and derivative discontinuity in density functional theory. *Advan. Quantum Chem.* 21:113-34, 1990.

4. Majewski J A & Vogl P. Self-interaction corrected density-functional formalism. I. Ground-state properties of the Hubbard-Peierls model. *Phys. Rev. B—Condensed Matter* 46:12219-34, 1992.

5. Svane A & Gunnarsson O. Transition-metal oxides in the self-interaction-corrected density-functional formalism. *Phys. Rev. Lett.* 65:1148-50, 1990.

6. Dreizler R M & Gross E K U. *Density-functional theory*. Berlin, Germany: Springer-Verlag, 1990. 302 p.

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