Errata

Erratum: Enhancing second-order nonlinear optical properties by controlling the wave function in one-dimensional conjugated molecules [Phys. Rev. B 40, 6292 (1989)]

Tetsuzo Yoshimura

All occurrences of the phrase "second-order hyperpolarizability" should be replaced with "first-order hyperpolarizability."

Erratum: Enhancement of the van der Waals energy between an atom and a cylindrical surface: Application to the edges of stepped surfaces [Phys. Rev. B 41, 1196 (1990)]

Yi-Chen Cheng and Jyh Shinn Yang

In order to be consistent with the definition of the density-response function in the planar surface case,[1] the right-hand side of Eq. (6) (definition of $\mathrm{Im}[D'(q,\omega)]$) should be multiplied by 2. Note that there is also a misprint. A factor $\rho\rho'$ should be inserted in the integrand of Eq. (6). With this definition of $\mathrm{Im}[D'(q,\omega)]$, the right-hand side of the van der Waals energy U_{cyl} in Eq. (8) is reduced by a factor of 2. With this correction, the enhancement of U_{cyl} near the edges of a stepped surface is qualitatively unchanged, however quantitatively the calculated enhancement factor is reduced by a factor of 2. For example, the enhancement factor is 2.1 instead of 4.2 for atom-surface separation at 4 a.u.

[1] Y.-C. Cheng and I. P. Tu (unpublished).

Erratum: Optimized pseudopotentials [Phys. Rev. B 41, 1227 (1990)]

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The calculation of the bulk properties of fcc copper was affected by a minor amount of self-consistency error during the course of finding the electronic wave functions. This effect was caused by eigenvalues crossing above or below the Fermi level on successive iterations. With the advent of conjugate-gradient methods,[1,2] which maintain self-consistency

between wave functions and charge density throughout the calculation, this effect has been eliminated. With this correction, Table II now reads as follows:

TABLE II. Comparison of the bulk properties of fcc copper as obtained by the present method of calculation to experimental values.

	Experiment	Present	% Difference
Lattice constant (a.u.)	6.81	6.82	+0.1
Cohesive energy (Ry/atom)	0.257	0.302	+17.5
Bulk modulus (Mbar)	1.42	1.53	+7.7

[1]M. P. Teter, M. C. Payne, and D. C. Allan, Phys. Rev. B **40**, 12 255 (1989).
[2]T. A. Arias, M. C. Payne, and J. D. Joannopoulos (unpublished).