

ERRATUM | JUNE 07 2006

Erratum: "Hybrid functionals based on a screened Coulomb potential" [J. Chem. Phys. 118, 8207 (2003)] ✓

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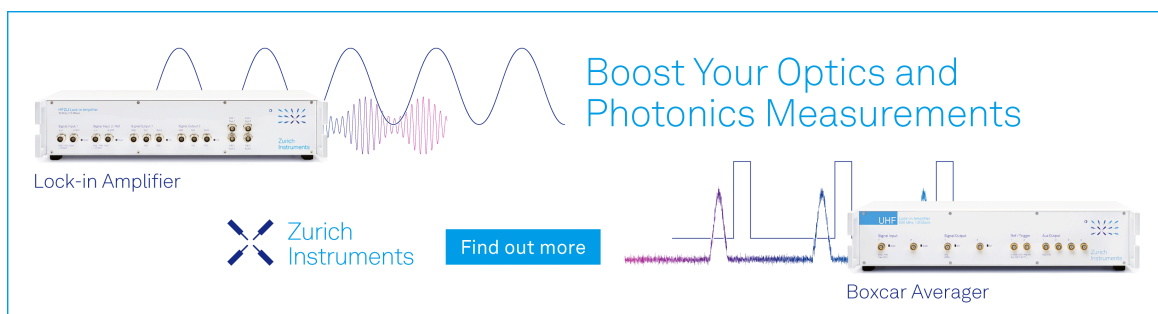


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**Erratum: “Hybrid functionals based on a screened Coulomb potential”
[J. Chem. Phys. **118**, 8207 (2003)]**Jochen Heyd and Gustavo E. Scuseria^{a)}*Department of Chemistry, Rice University, Houston, Texas 77005-1892*

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The screening parameter quoted in this paper ($\omega=0.15$) is not the one that was actually used in the code. In order to reproduce our results, two ω values are needed: $\omega = 0.15/\sqrt{2} \approx 0.106$ for Hartree-Fock and $\omega = 0.15 \times 2^{1/3} \approx 0.189$ for the PBE part.

This erratum applies to all of our ω PBEh and HSE calculations published to date. We emphasize, however, that all

our results obtained with this functional are reproducible using the two ω values quoted above. The validity of all our published HSE values is not affected.

Optimization of a single value of ω for a functional of the type reported in this paper will be presented elsewhere. We thank Oleg Vydrov and Artur Izmaylov for finding this error.

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