

Correction to "Multiconfiguration Pair-Density Functional Theory Spectral Calculations Are Stable to Adding Diffuse Basis Functions"

Chad E. Hoyer, Laura Gagliardi,* and Donald G. Truhlar*

J. Phys. Chem. Lett. 2015, 6 (21), 4181-4188. DOI: 10.1021/acs.jpclett.5b01888

Supporting Information

We found a small error in the code used in the computation of tPBE values. This results in minor changes in some nonsinglet excitation energies and does not change any conclusions in the Letter. The changes in the total energies and excitation energies are in the Supporting Information of this Addition/Correction.

ASSOCIATED CONTENT

S Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.jpclett.5b02661.

Tables from the original Letter are presented with updated tPBE values (PDF)

AUTHOR INFORMATION

Corresponding Authors

*E-mail: gagliard@umn.edu (L.G.). *E-mail: truhlar@umn.edu (D.G.T).

