Publisher’s Note: “Derivative couplings between TDDFT excited states obtained by direct differentiation in the Tamm-Dancoff approximation” [J. Chem. Phys. 141, 024114 (2014)]

Shervin Fatehi
University of Texas Rio Grande Valley, shervin.fatehi@utrgv.edu

Follow this and additional works at: https://scholarworks.utrgv.edu/chem_fac

Part of the Chemistry Commons

Recommended Citation
Publisher’s Note: “Derivative couplings between TDDFT excited states obtained by direct differentiation in the Tamm-Dancoff approximation” [J. Chem. Phys. 141, 024114 (2014)]

Qi Ou,1 Shervin Fatehi,1,a) Ethan Alguire,1 Yihan Shao,2 and Joseph E. Subotnik1,b)
1Department of Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA
2Q-Chem, Inc., 6601 Owens Drive, Suite 105, Pleasanton, California 94588, USA

(Received 14 July 2014; published online 12 August 2014)

[http://dx.doi.org/10.1063/1.4891539]

This article was originally published online on 14 July 2014 with the following errors:
1. A notation was omitted in Reference 84. This error was corrected in all online versions of the article on 15 July 2014; the reference is correct as it appears in the printed version of the journal.
2. There were several errors in Eqs. (7) and (15). Equation (7) should be

\[ \mathcal{O}_{\text{KS}} = \sum_{pq} F_{pq} a_p^\dagger a_q 
+ \sum_{cdkl} [\Omega_{cilkd} a_c^\dagger a_l^\dagger a_d^\dagger a_k + \Omega_{cdkl} (a_c^\dagger a_k^\dagger a_d^\dagger a_l^\dagger)] , \]  

and Eq. (15) should be

\[ \mathcal{O}_{\text{KS}} = \sum_{pq} \left( h_{pq}^0 + g_{pq} + \sum_m \Pi_{pqm} \right) a_p^\dagger a_q 
+ \sum_{cdkl} [\Pi_{cilkd} + \omega_{cilkd} a_c^\dagger a_l^\dagger a_d a_k 
+ (\Pi_{cdkl} + \omega_{cdkl}) (a_c^\dagger a_k^\dagger a_d a_l^\dagger) ] . \]  

These errors were corrected in all online versions of the article on 25 July 2014. AIP Publishing apologizes for these errors.

a)Present address: Department of Chemistry and Henry Eyring Center for Theoretical Chemistry, University of Utah, 315 South 1400 East, Salt Lake City, Utah 84103, USA.
b)Electronic mail: subotnik@sas.upenn.edu