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SUPPLEMENTAL ONLINE MATERIAL

Performance of SOPPA based methods in the calculation of vertical excitation energies and oscillator strengths

Stephan P. A. Sauer[a†], Henrik F. Pitzner-Frydendahl[a], Mogens Buse[b], Hans Jørgen Aa. Jensen[b‡], and Walter Thiel[c*]

[a]*Department of Chemistry, University of Copenhagen, DK-2100 Copenhagen Ø, Denmark*; [b]*Department of Physics, Chemistry and Pharmacy, University of Southern Denmark, DK-5230 Odense M, Denmark*; [c]*Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, D-45470 Mülheim an der Ruhr, Germany*

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In this supplemental online material we present the statistical analysis of the comparison between the results from the RPA(D), SOPPA(SOS-MP2), SOPPA, SOPPA(SCS-MP2), SOPPA(CCSD) calculations and the CASPT2 calculations for both the TZVP and aug-cc-pVTZ basis sets.

†Corresponding author. Email: sauer@kiku.dk
†Email: hjj@sdu.dk
*Corresponding author. Email: thiel@mpi-muelheim.mpg.de

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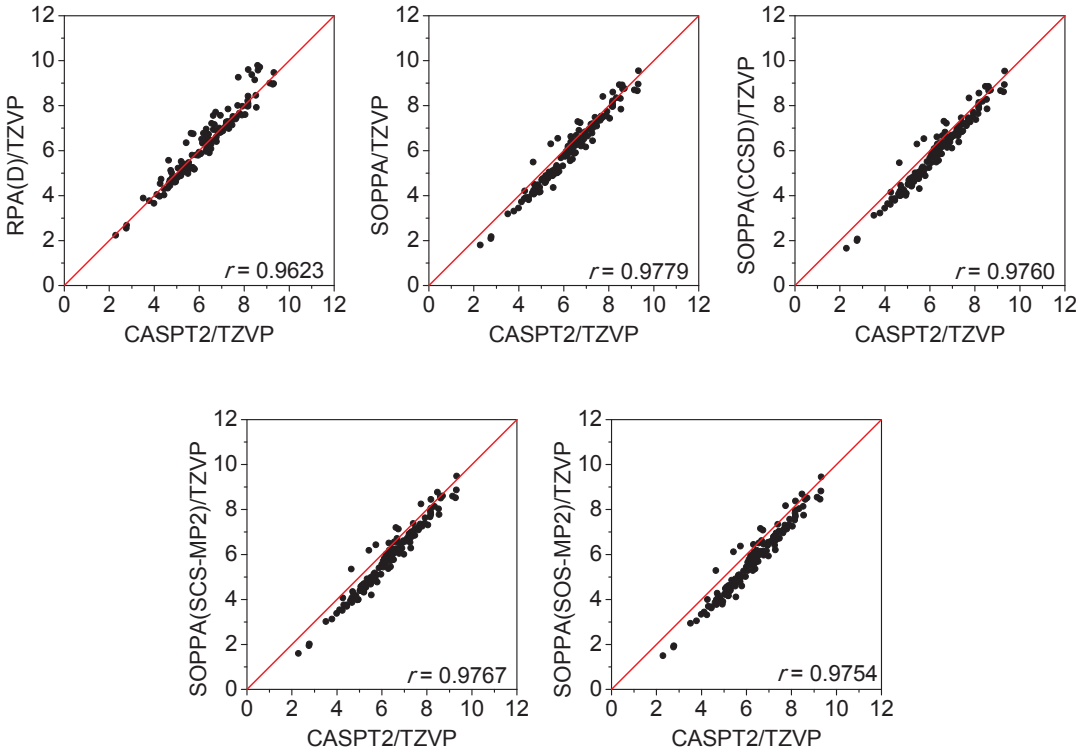

Figure 1. Correlation plots for the vertical excitation energies (eV) of singlet excited states with the TZVP basis set: RPA(D), SOPPA, SOPPA(CCSD) and SOPPA(SCS-MP2), SOPPA(SOS-MP2) vs. CASPT2 results.

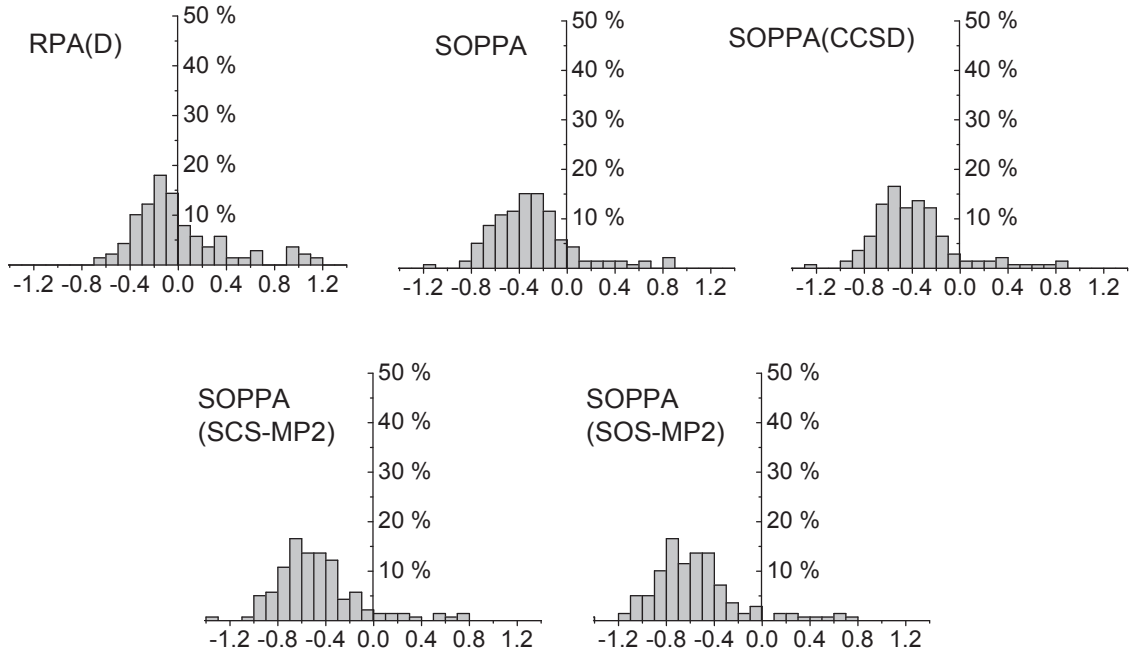

Figure 2. Histograms (in %) of the deviations between RPA(D), SOPPA, SOPPA(CCSD), SOPPA(SCS-MP2), SOPPA(SOS-MP2) and CASPT2 vertical excitation energies (eV) of singlet excited states calculated with the TZVP basis set.

Table 1. Deviations in the vertical excitation energies (eV) of singlet excited states with the TZVP basis set from the CASPT2/TZVP results[a].

	RPA(D)	SOPPA	SOPPA(SCS-MP2)	SOPPA(SOS-MP2)	SOPPA(CCSD)
Count[b]	139	139	139	139	139
Mean	0.03	-0.28	-0.46	-0.55	-0.37
Abs. Mean	0.31	0.38	0.53	0.61	0.46
Std. Dev.	0.42	0.34	0.35	0.36	0.35
Maximum (+)	1.52	0.88	0.76	0.70	0.87
Maximum (−)	0.62	1.17	1.33	1.42	1.22

[a] TZVP results from Refs. [1].

[b] Total number of considered states.

Table 2. Deviations in the vertical excitation energies (eV) of singlet excited states with the aug-cc-pVTZ basis set from the CASPT2 set of results[a].

	RPA(D)	SOPPA	SOPPA(CCSD)
Count[b]	117	117	117
Mean	-0.07	-0.37	-0.49
Abs. Mean	0.41	0.47	0.58
Std. Dev.	0.55	0.37	0.39
Maximum (+)	2.59	1.52	1.44
Maximum (−)	1.43	1.08	1.14

[a] Results from Ref.[2].

[b] Total number of considered states.

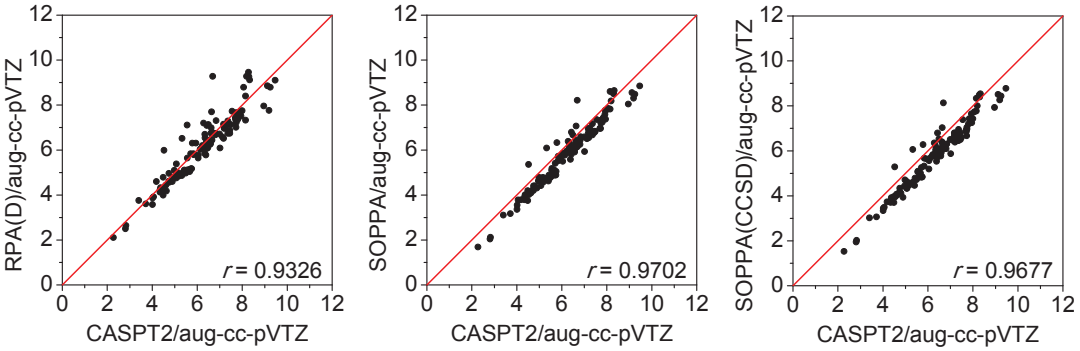

Figure 3. Correlation plots for the vertical excitation energies (eV) of singlet excited states with the aug-cc-pVTZ basis set: RPA(D), SOPPA and SOPPA(CCSD) vs. CASPT2 results.

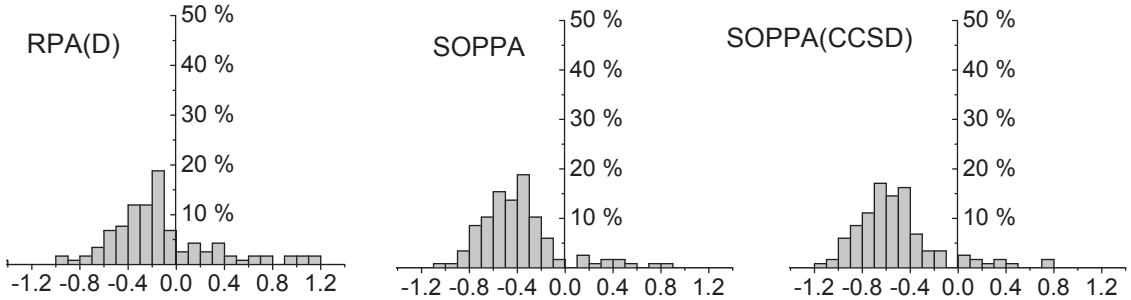

Figure 4. Histograms (in %) of the deviations between RPA(D), SOPPA, SOPPA(CCSD) and CASPT2 vertical excitation energies (eV) of singlet excited states calculated with the aug-cc-pVTZ basis set.

References

[1] M.R. Silva-Junior, M. Schreiber, S.P.A. Sauer and W. Thiel, Benchmarks for electronically excited states: TD-DFT and DFT/MRCI, J. Chem. Phys. **129**, 104103 (2008).

[2] M.R. Silva-Junior, M. Schreiber, S.P.A. Sauer and W. Thiel, Benchmarks of electronically excited states: Basis set effects on CASPT2 results, J. Chem. Phys. **133**, 174318 (2010).