Supporting information to "Self-Consistent Implementation of Kohn-Sham Adiabatic Connection Models with Improved Treatment of the Strong-Interaction Limit"

Szymon Śmiga[a], Fabio Della Sala[b,c], Paola Gori-Giorgi[d], Eduardo Fabiano[b,c]

[a] *Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudziadzka 5, 87-100 Torun, Poland*

[b] *Institute for Microelectronics and Microsystems (CNR-IMM), Via Monteroni, Campus Unisalento, 73100 Lecce, Italy*

[c] *Center for Biomolecular Nanotechnologies@UNILE, Istituto Italiano di Tecnologia (IIT), Via Barsanti, 73010 Arnesano (LE), Italy*

[d] *Department of Chemistry & Pharmaceutical Sciences and Amsterdam Institute of Molecular and Life Sciences (AIMMS), Faculty of Science, Vrije Universiteit, De Boelelaan 1083, 1081HV Amsterdam, The Netherlands,*

E-mail: szsmiga@fizyka.umk.pl

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1 Summary of the basis sets

- **He, He_2**: even tempered $20s10p2d$ basis.
- **Be, Ne, Ne_2**: uncontracted ROOS-ATZP basis[1].
- **Mg**: uncontracted aug-cc-pVTZ basis set[2].
- **Ar**: s and p basis functions from the uncontracted ROOS-ATZP[1] basis set and d and f functions from the uncontracted aug-cc-pwCVQZ basis set[3].
- **HF, CO, H_2O, H_2, Cl_2, N_2, HCl, NH_3 , C_2H_6**: uncontracted cc-pVTZ basis set of Dunning[4].

2 Dissociation of H_2 with SPL functional

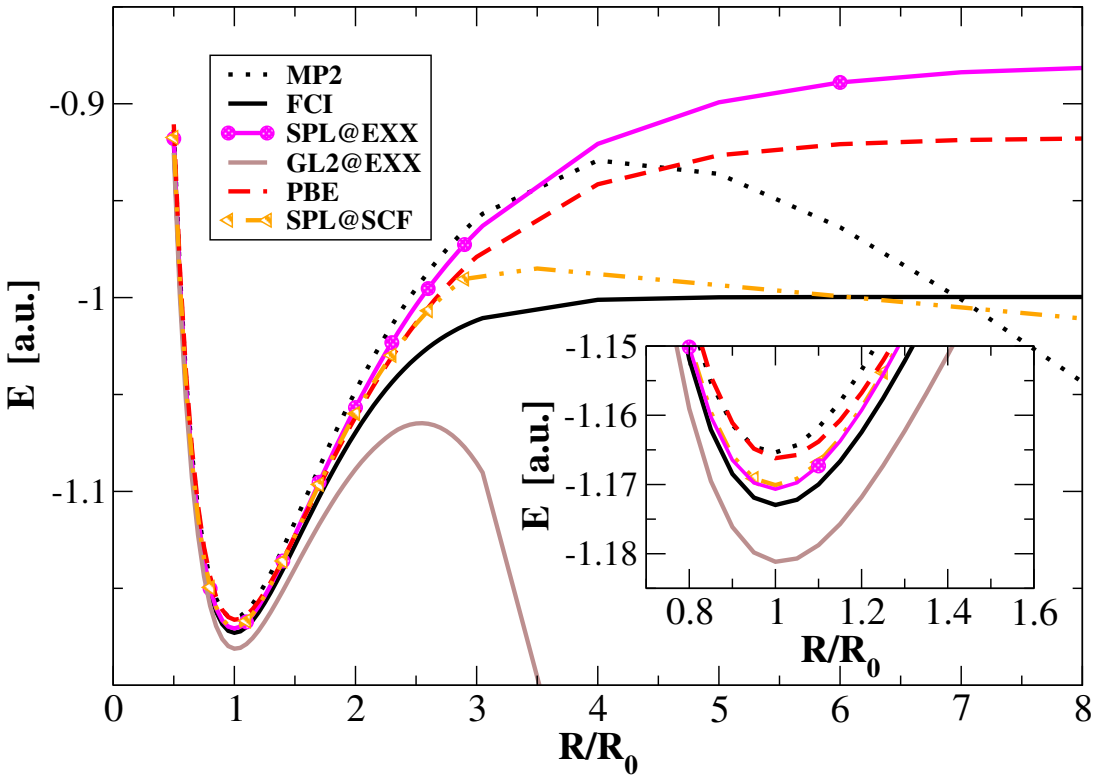

Figure S1: The total energy of the H_2 molecule as it is stretched calculated with the various methods. The inset presents the same data around the equilibrium distance.

3 Hookes atom results

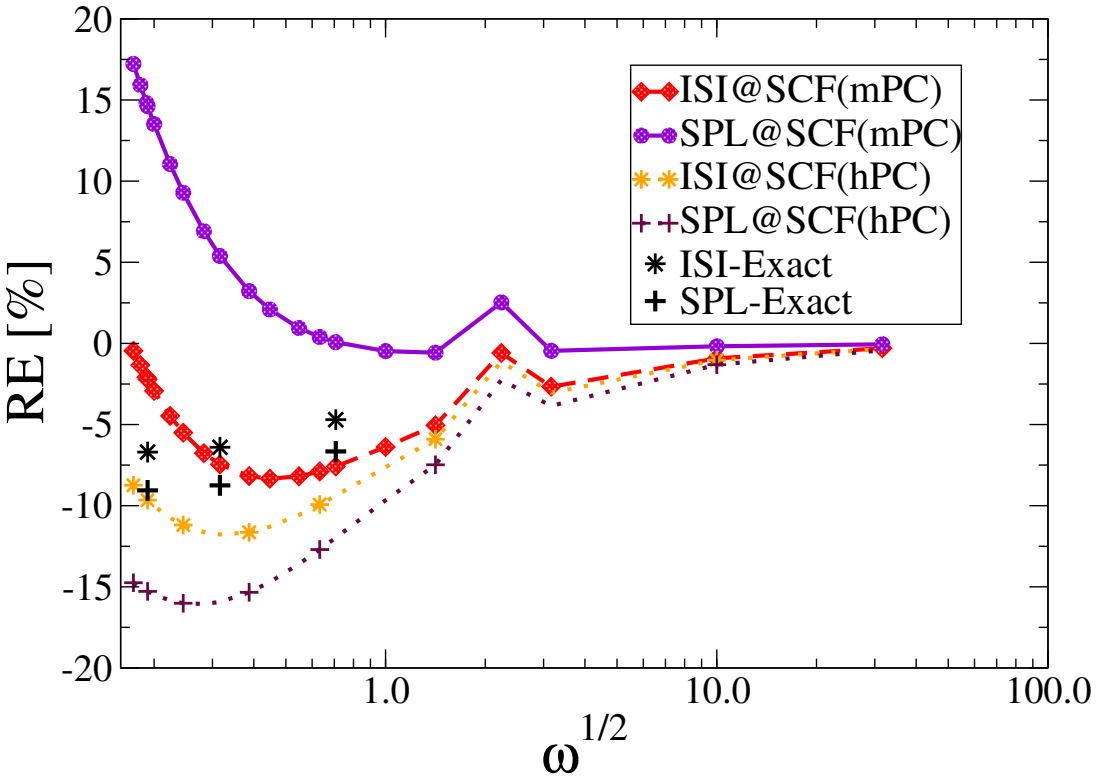

Figure S2: Relative error on correlation energies of harmonium atoms for various values of ω computed at @SCF orbitals for ISI and SPL functionals using the hPC and mPC models for the strong-interaction functionals. The errors have been computed with respect FCI data obtained in the same basis set[5]. The exact ISI and SPL values are taken from Ref.[6], and are obtained by inserting exact densities into the ISI and SPL functionals, including the exact treatment (SCE) of the strong-interaction limit.

References

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