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

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1 Summary of the basis sets

- **He, He**: even tempered 20s10p2d basis.

- **Be, Ne, Ne**: 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\(_2\)O, H\(_2\), Cl\(_2\), N\(_2\), HCl, NH\(_3\), C\(_2\)H\(_6\)**: uncontracted cc-pVTZ basis set of Dunning\(^4\).

2 Dissociation of H\(_2\) with SPL functional

![Graph](image)

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.
Figure S2: Relative error on correlation energies of harmonium atoms for various values of $\omega$ 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. The exact ISI and SPL values are taken from Ref., and are obtained by inserting exact densities into the ISI and SPL functionals, including the exact treatment (SCE) of the strong-interaction limit.
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