

# Supplementary Information for “Basis-set correction based on density-functional theory: Linear-response formalism for excited-state energies”

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For each basis set  $\mathcal{B}$  of size  $n_{\max}$ , the LDA basis-set correction energy per particle is fitted to a rational fraction

$$\bar{\epsilon}^{\mathcal{B}}(\rho) \approx \frac{\sum_{i=0}^4 a_i^{\mathcal{B}} \rho^i}{1 + \sum_{j=1}^4 b_j^{\mathcal{B}} \rho^j}, \quad (1)$$

where the coefficients are given in Tab. I.

TABLE I: Coefficients for the rational fraction of Eq. (1) in Hartree atomic units. The coefficients have been found using Mathematica NonlinearModelFit function.

$n_{\max}$	$a_0^{\mathcal{B}}$	$a_1^{\mathcal{B}}$	$a_2^{\mathcal{B}}$	$a_3^{\mathcal{B}}$	$a_4^{\mathcal{B}}$	$b_1^{\mathcal{B}}$	$b_2^{\mathcal{B}}$	$b_3^{\mathcal{B}}$	$b_4^{\mathcal{B}}$
1	-0.000071	-0.198377	-4.150011	14.507548	-21.949820	20.296972	139.231729	-321.276975	536.780361
2	-0.000594	-0.173014	0.384433	-0.244367	-0.365982	5.401147	-7.446688	6.256052	8.969527
3	0.000444	-0.330837	0.297792	0.012509	-0.652327	24.748701	-18.057894	4.452590	15.604104
4	0.000795	-0.483374	0.382824	-0.346615	-0.485469	50.965472	-37.484558	17.394304	11.199767
5	0.000879	-0.637201	0.012849	0.251293	-0.793912	82.954134	-50.063365	9.142699	18.248454
10	-0.005058	0.025411	-0.076797	0.085669	-0.034448	-2.385101	3.352381	-2.446328	0.874405
20	-0.003546	0.018777	-0.073303	0.062172	-0.018124	-0.362275	1.663291	-1.437415	0.436582
30	-0.001524	-0.001298	-0.003401	0.004565	-0.001330	-1.064542	0.542581	-0.183654	0.036448
40	-0.001315	-0.001846	-0.000559	0.001925	-0.000579	-1.045314	0.447844	-0.113278	0.017638
50	-0.001259	-0.001685	0.000160	0.001096	-0.000349	-1.036763	0.413128	-0.088704	0.011676
60	-0.001212	-0.001615	0.000544	0.000651	-0.000229	-1.015071	0.382952	-0.073090	0.008439
70	-0.002015	0.026366	-0.069143	-0.167102	-0.010058	-10.127259	52.123001	-7.934000	0.982991

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