Supporting Information for: "Simultaneous benchmarking of ground- and excited-state properties with long-range-corrected density functional theory" [*J. Chem. Phys.* **129**, 034107 (2008)]

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Table 1: Carbon Monoxide excitation energies for various basis sets. LRC-PBE, $\mu = 0.300$ a_0^{-1} .

6-31+G(d)	6-311++G(d,p)	aug-cc-pvdz	aug-cc-pvtz	aug-cc-pvtz - aug-cc-pvdz
5.8878	5.8878	5.8714	5.8545	-0.02
5.8878	5.8878	5.8714	5.8545	-0.02
8.1855	8.1855	8.1694	8.1714	0.00
8.4503	8.4503	8.4206	8.4032	-0.02
8.4503	8.4503	8.4206	8.4033	-0.02
8.9323	8.9323	8.9035	8.8799	-0.02
8.9324	8.9324	8.9036	8.8801	-0.02
9.8833	9.8833	9.8722	9.8684	0.00
9.8833	9.8833	9.8722	9.8684	0.00
10.058	10.0582	10.0811	9.9743	-0.11
10.395	10.395	10.3789	10.3483	-0.03
10.3951	10.3951	10.379	10.3484	-0.03
10.8087	10.8087	10.7377	10.66	-0.08
10.8397	10.8397	10.7921	10.6621	-0.13
11.1385	11.1385	11.0153	10.8696	-0.15
11.1385	11.1385	11.0153	10.8696	-0.15
11.206	11.206	11.0606	10.8873	-0.17
11.4193	11.4193	11.2601	11.075	-0.19
11.4193	11.4193	11.2601	11.075	-0.19
11.8125	11.8125	11.8485	11.7754	-0.07
11.8125	11.8125	11.8485	11.7754	-0.07
12.8838	12.8838	12.8371	12.7407	-0.10
12.8838	12.8838	12.8371	12.7407	-0.10
13.041	13.041	12.9996	12.8928	-0.11
13.041	13.041	12.9996	12.8928	-0.11
13.7396	13.7396	13.5507	13.1301	-0.42
13.8314	13.8314	13.7229	13.1991	-0.52
13.8316	13.8316	13.782	13.5965	-0.19
14.0806	14.0806	13.782	13.5967	-0.19
14.1959	14.1959	14.1123	13.8431	-0.27

Table 2: Uracil excitation energies for various basis sets. Using the geometry from Taylor and Kennard, J.Am.Chem.Soc. vol.104 p.3209 (1982). LRC-PBE, $\mu = 0.300 \;\; a_0^{-1}$.

6-31+G(d)	6-311++G(d,p)	aug-cc-pvdz	aug-cc-pvtz	aug-cc-pvtz - aug-cc-pvdz
3.4539	3.4473	3.4322	3.4235	-0.01
4.4095	4.3957	4.365	4.3635	0.00
4.8742	4.8605	4.8216	4.8186	0.00
4.972	4.9699	4.9398	4.9432	0.00
5.4927	5.4845	5.3749	5.3766	0.00
5.6044	5.6034	5.569	5.5748	0.01
5.7783	5.7657	5.7184	5.7215	0.00
6.1838	6.1717	6.1118	6.1134	0.00
6.2883	6.282	6.2535	6.2469	-0.01
6.5063	6.3797	6.3495	6.3789	0.03
6.5243	6.5134	6.4342	6.4318	0.00
6.8789	6.8665	6.7865	6.7971	0.01

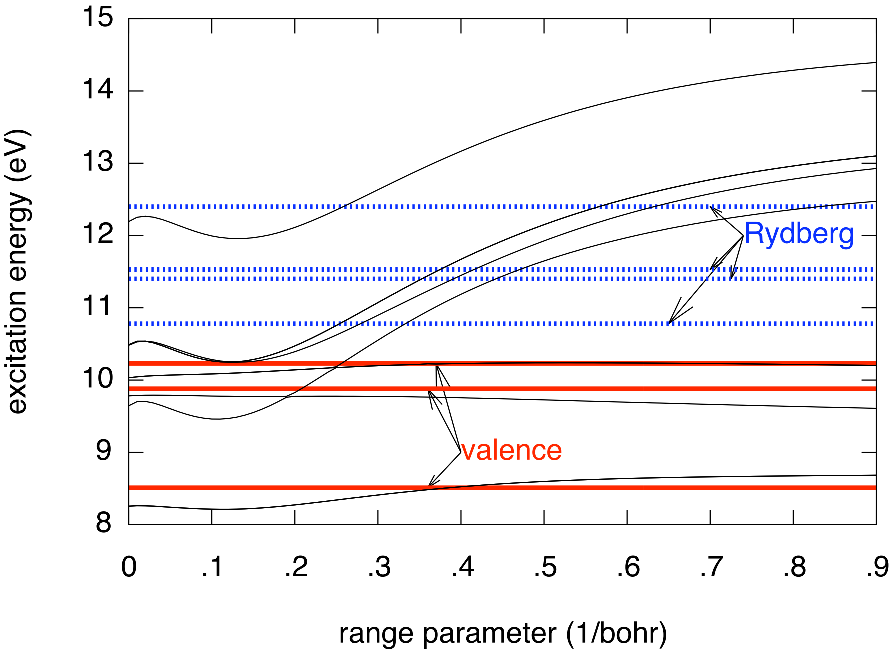

Figure 1: Excitation energies for carbon monoxide with LRC-BLYP.

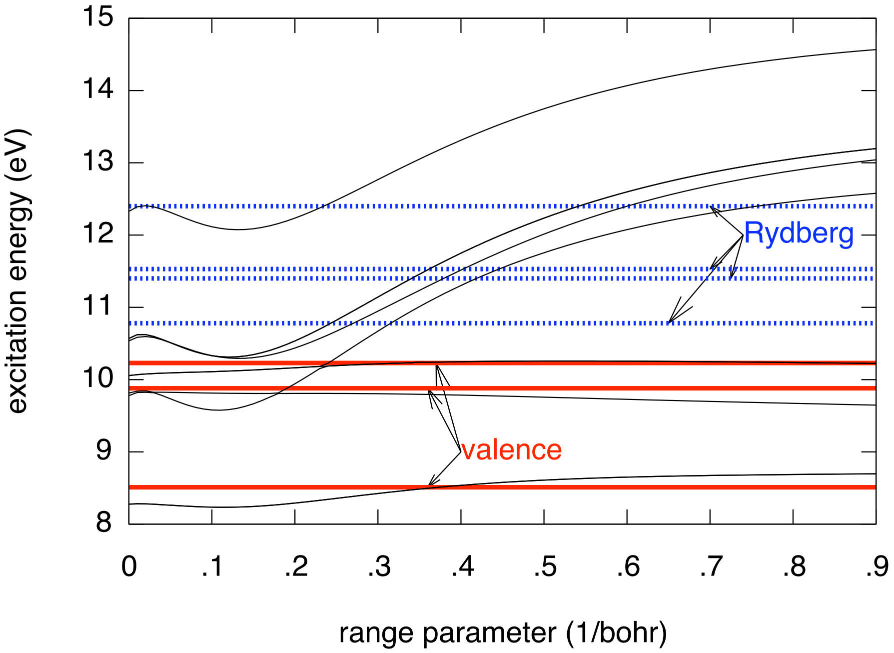

Figure 2: Excitation energies for carbon monoxide with LRC-BOP.

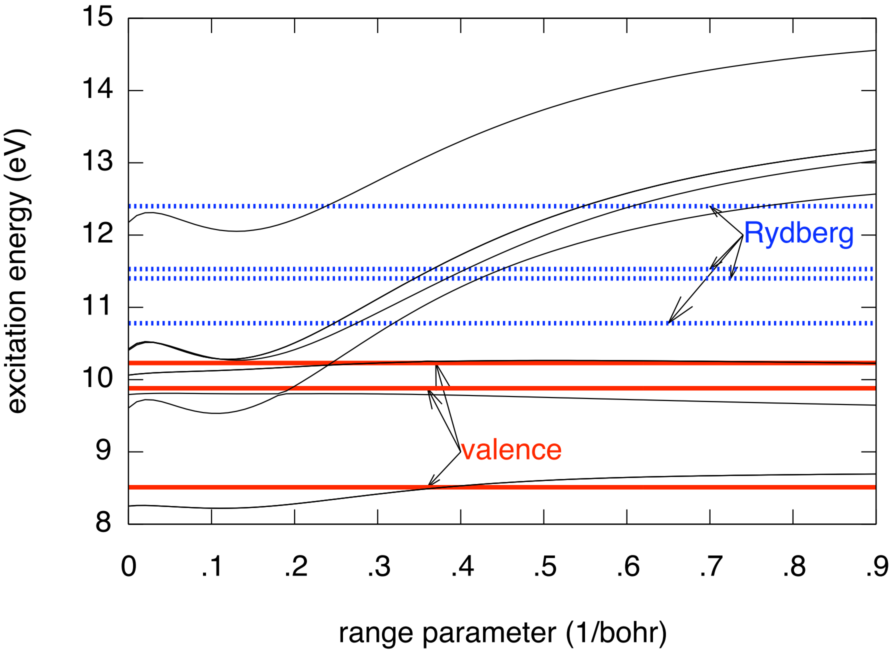

Figure 3: Excitation energies for carbon monoxide with LRC-PBEOP.

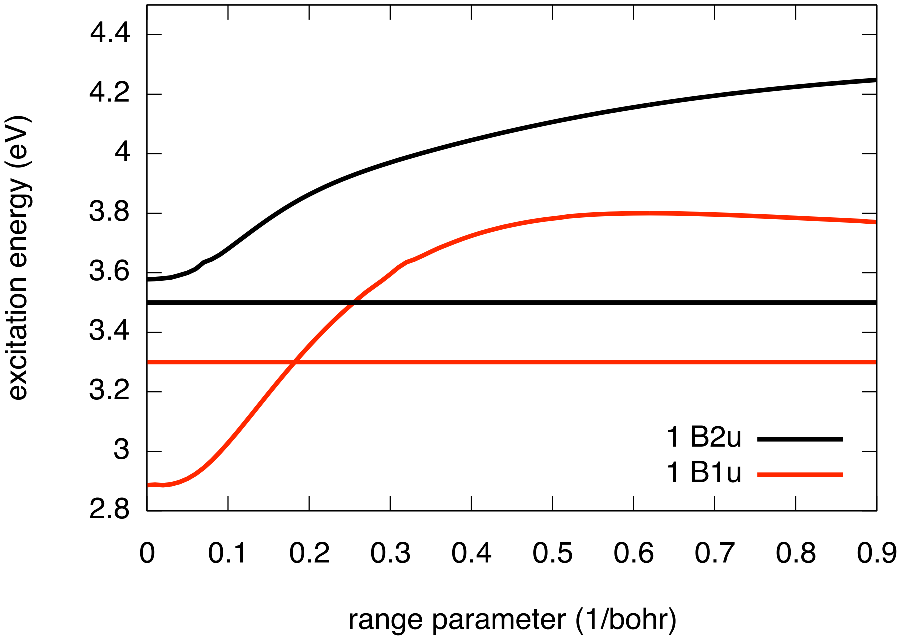

Figure 4: Excitation energies for anthracene with LRC-BLYP. The horizontal lines correspond to the experimental estimate, while the curved lines are the calculation.

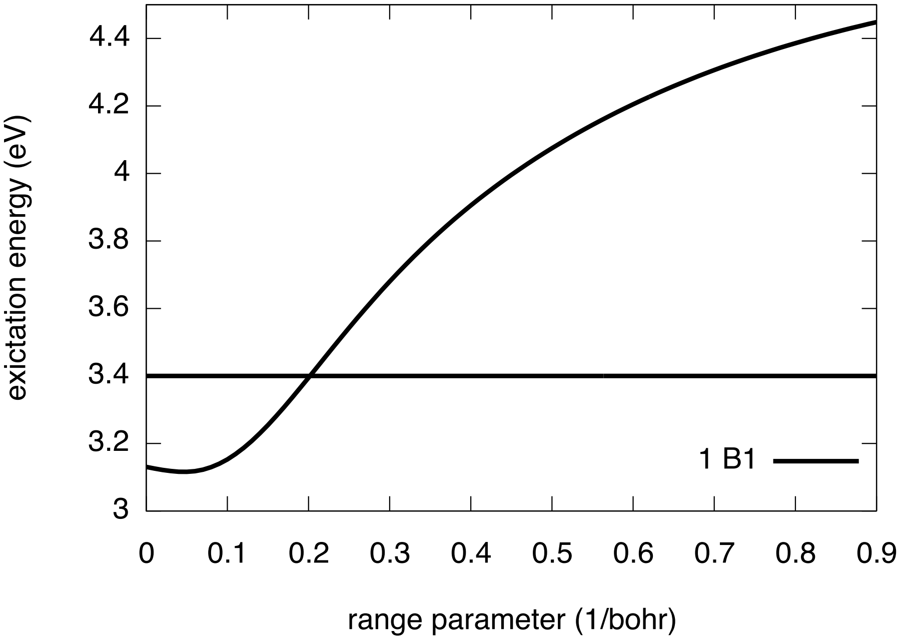

Figure 5: Excitation energies for pyridazine with LRC-BLYP. The horizontal line corresponds to the experimental estimate, while the curved line is the calculation.

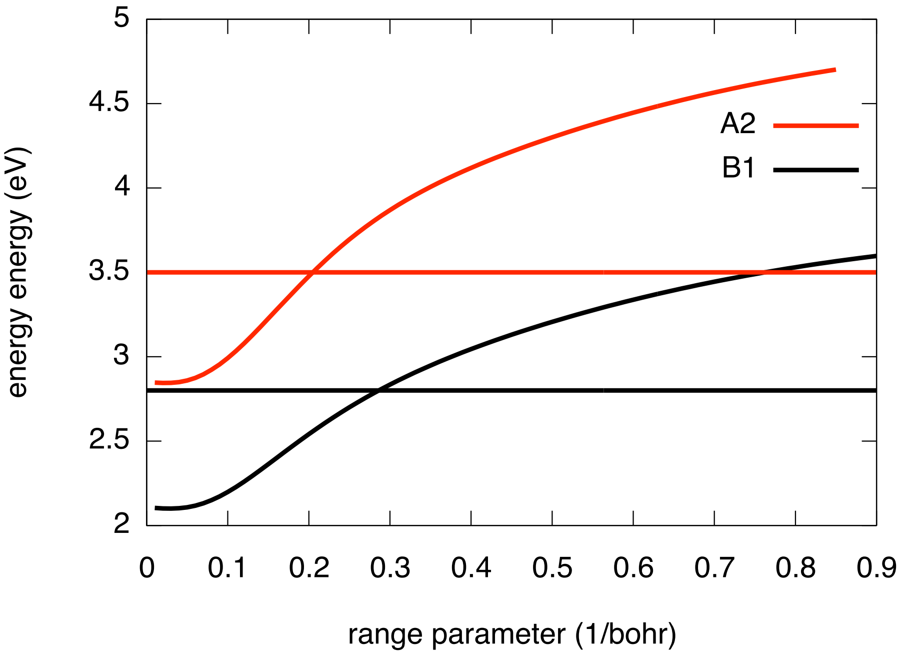

Figure 6: Excitation energies for benzocyclobutenedione with LRC-BLYP. The horizontal lines correspond to the experimental estimate, while the curved lines are the calculation.

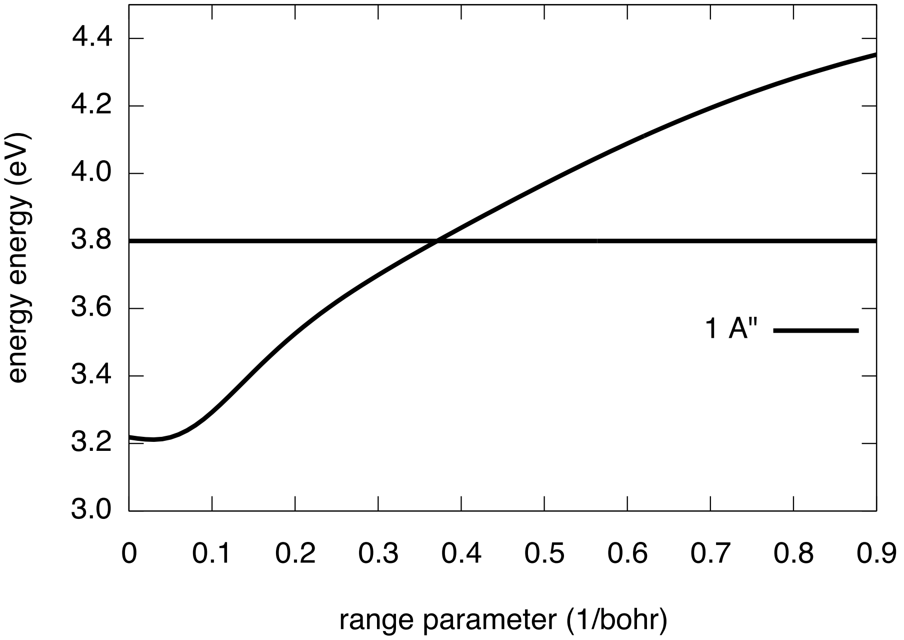

Figure 7: Excitation energies for benzaldehyde with LRC-BLYP. The horizontal line corresponds to the experimental estimate, while the curved line is the calculation.

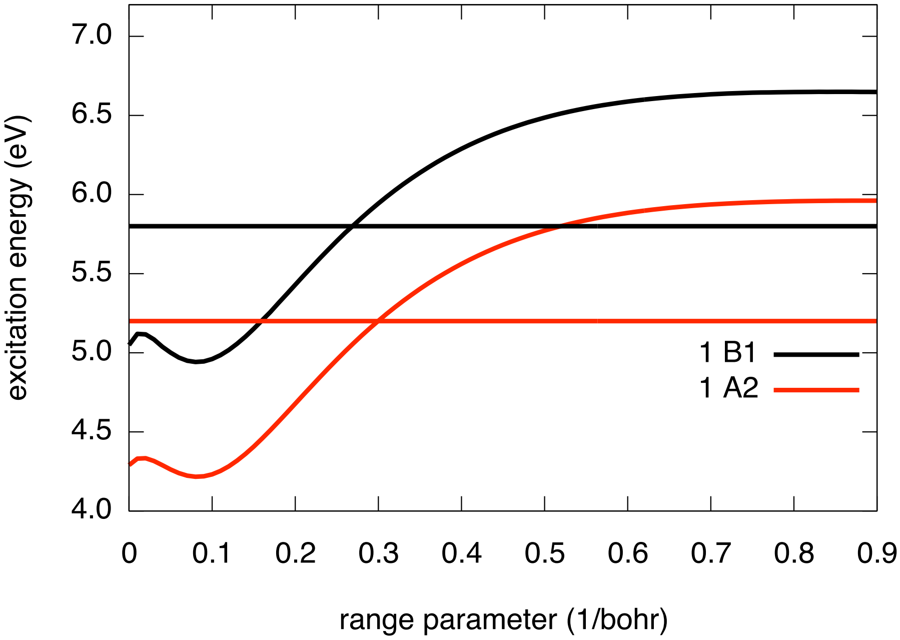

Figure 8: Excitation energies for pyrrole with LRC-BLYP. The horizontal lines correspond to the experimental estimate, while the curved lines are the calculation.

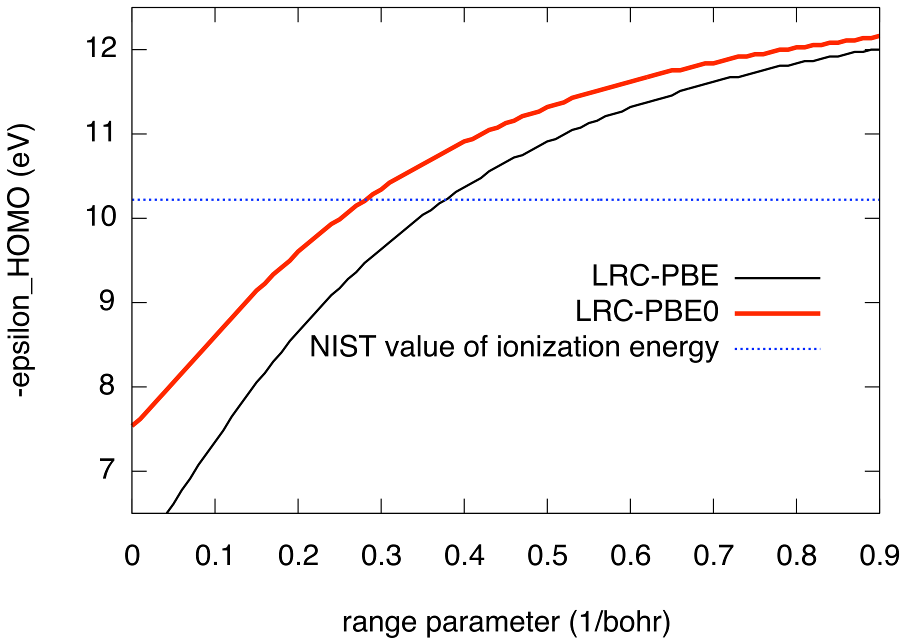

Figure 9: $-\varepsilon_{\mathrm{HOMO}}$ for acetaldehyde.

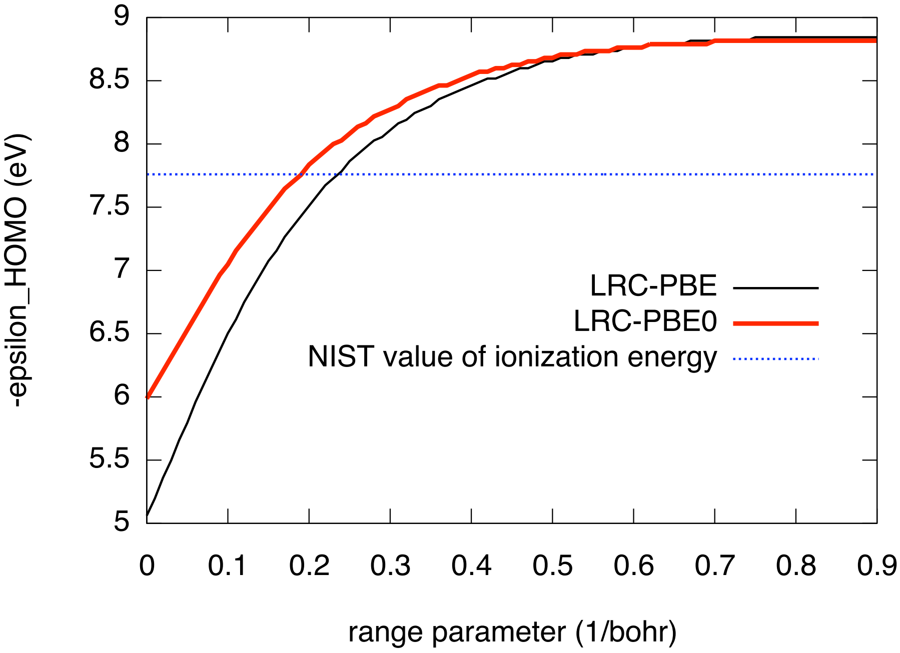

Figure 10: $-\varepsilon_{\text{HOMO}}$ for indole.

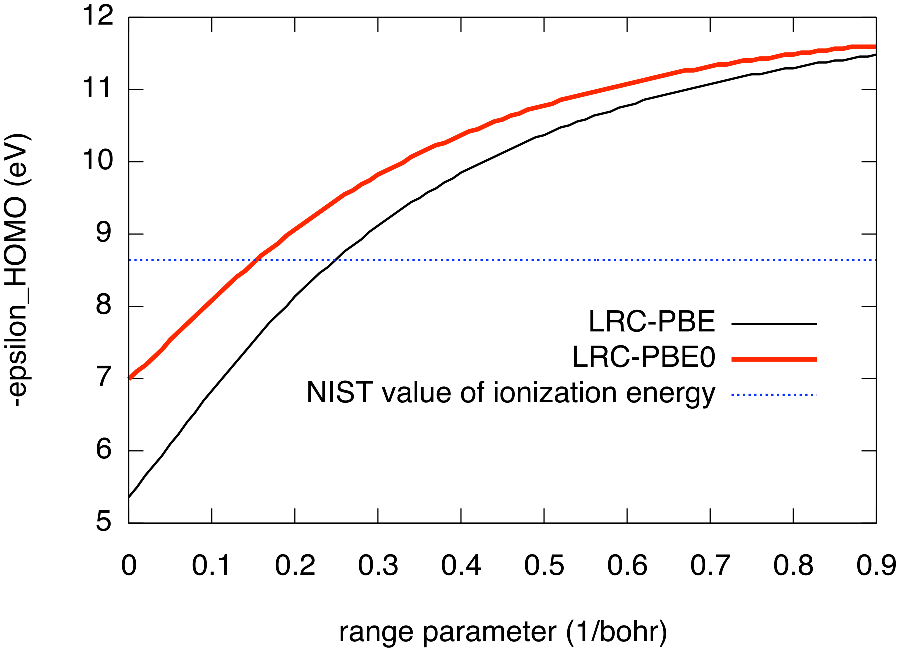

Figure 11: $-\varepsilon_{\mathrm{HOMO}}$ for pyridazine.

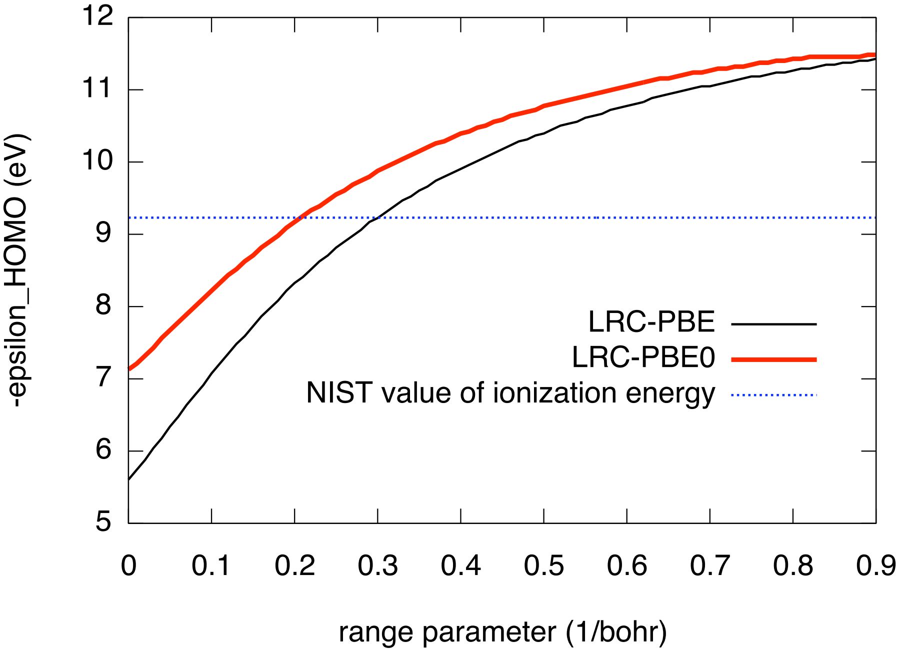

Figure 12: $-\varepsilon_{\text{HOMO}}$ for benzocyclobutenedione.

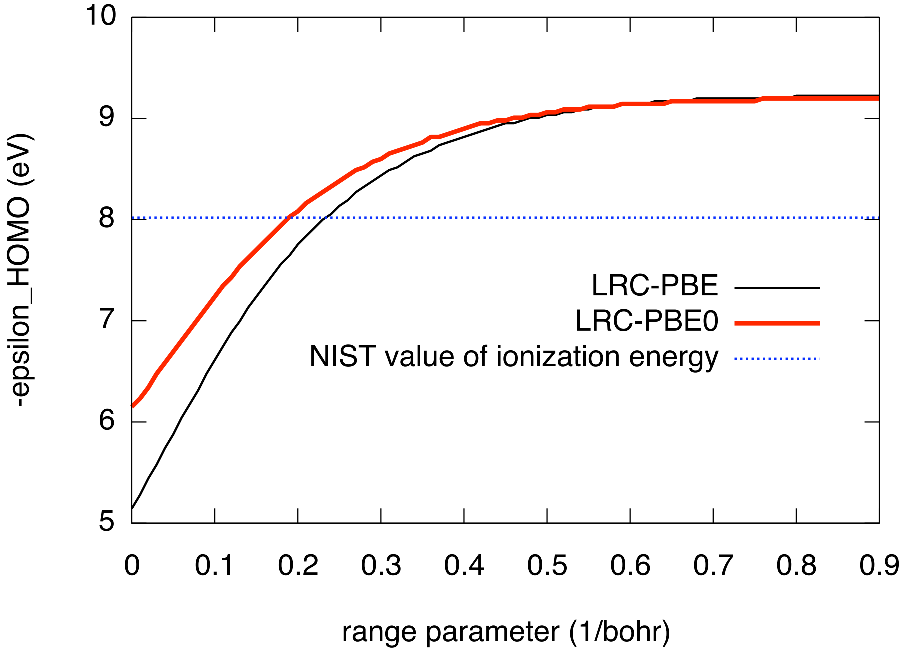

Figure 13: $-\varepsilon_{\text{HOMO}}$ for pyrrole.