

Supplementary materials

Library of dispersion corrected atom centered potentials for generalized gradient approximation functionals: elements H, C, N, O, He, Ne, Ar and Kr

I-C. Lin, M. D. Coutinho-Neto, C. Felsenheimer, O. A. von Lilienfeld, I. Tavernelli and U. Rothlisberger

	(H ₂) ₂	(Benzene) ₂	(N ₂) ₂	(CO ₂) ₂
$E_{\min}^{\text{DCACP}} / r_{\min}^{\text{DCACP}}$	-0.05 / 3.6	-1.72 / 3.9	-0.19 / 3.8	-0.47 / 3.4
$E_{\min}^{\text{Ref}} / r_{\min}^{\text{Ref}}$	-0.04 / 3.4	-1.70 / 3.9	-0.20 / 3.8	-0.46 / 3.3
Reference level	Full CI	CCSD(T) aug-ccpVQZ	CCSD(T) aug-ccpVTZ	CCSD(T) aug-ccpVTZ

Table 1: Configurations of the calibration systems and their corresponding equilibrium distance and energy (E_{\min}^{Ref} , r_{\min}^{Ref}). The performance of DCACPs are also tabulated (E_{\min}^{DCACP} , r_{\min}^{DCACP}). r in Å and E in kcal/mol.

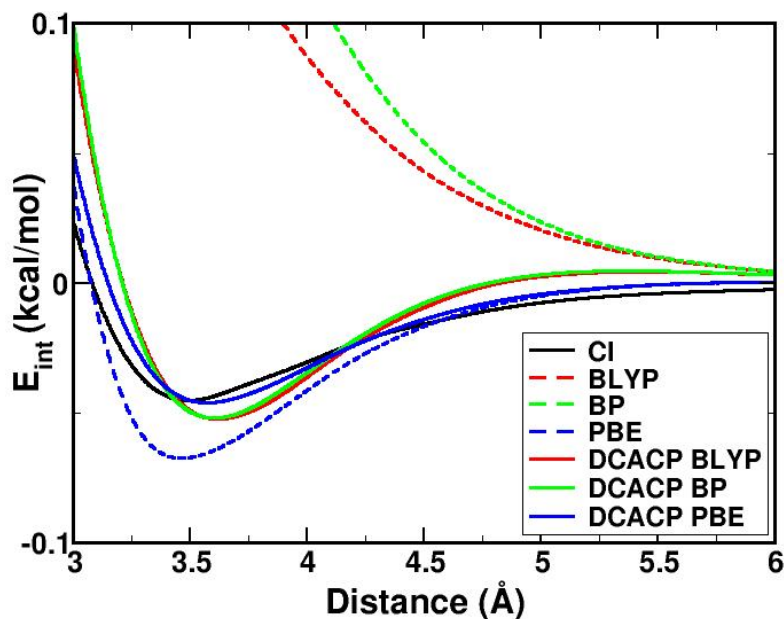


Figure 1: Calibration of hydrogen: interaction energy curve of the parallel H₂ dimer as a function of intermolecular distance. CI reference taken from H. Lavendry *et al. Chem. Phys. Lett.*, **196**, 377, (1992).

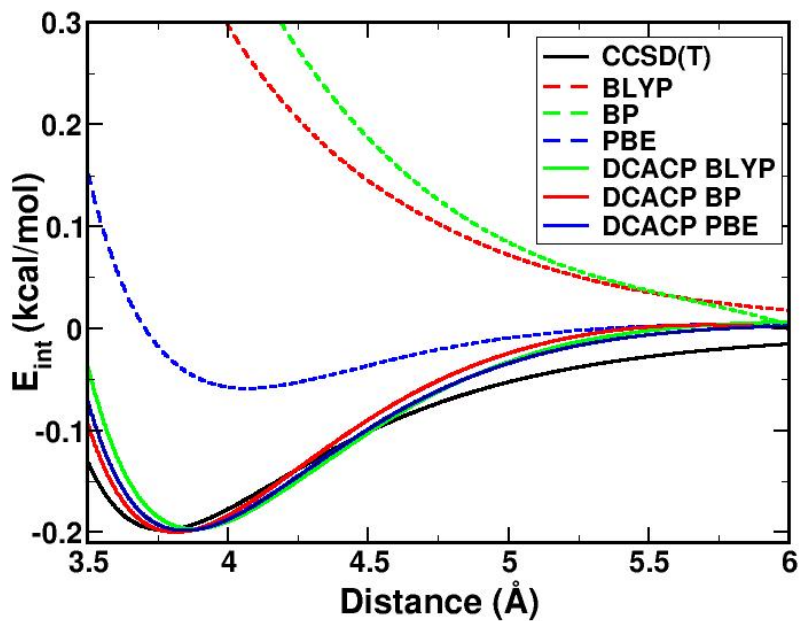


Figure 2: Calibration of nitrogen: interaction energy curve of the parallel N_2 dimer as a function of intermolecular distance.

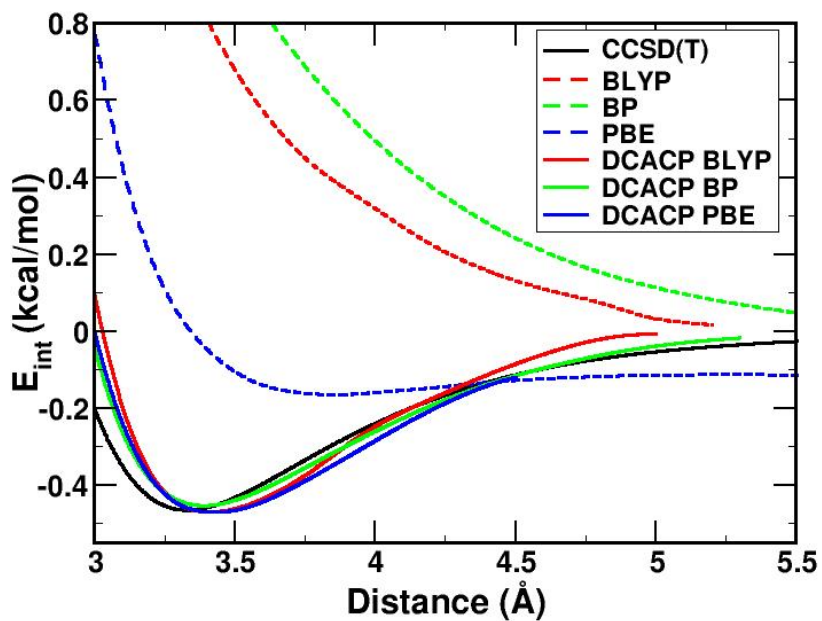


Figure 3: Calibration of oxygen: interaction energy curve of the CO_2 dimer in cross shape as a function of intermolecular distance.

	He		Ne		Ar		Kr	
	E_{\min}	r_{\min}	E_{\min}	r_{\min}	E_{\min}	r_{\min}	E_{\min}	r_{\min}
BLYP	0.020	3.0	0.094	3.0	0.247	3.8	0.322	4.2
BP	0.022	3.1	0.105	3.2	0.250	3.8	0.322	4.2
PBE	0.021	3.0	0.077	3.2	0.248	3.8	0.317	4.2
Ref.	0.020	3.0	0.082	3.2	0.249	3.8	0.322	4.2

Table 2: Calibration of rare gas atoms: equilibrium interaction energy (E_{\min} , kcal/mol) and distance (r_{\min} , Å) of rare gas dimers. All functionals are complemented with DCACPs. Ref. is taken from N. Kurita and H. Sekino, *Int. J. Quantum Chem.*, **91**, 355, (2003).

	H ₂	C ₆ H ₆		N ₂	CO ₂
	r_{HH}	r_{CH}	r_{CC}	r_{NN}	r_{CO}
BLYP	0.747	1.087	1.400	1.100	1.171
DCACP	0.747	1.087	1.400	1.100	1.171

Table 3: Bond lengths (Å) of the optimized isolated monomers in the calibration system calculated with both uncorrected and DCACP-augmented BLYP functional.

H ₂		H ₂ O		CO ₂	
DCACP	BLYP	DCACP	BLYP	DCACP	BLYP
4566.917	4568.419	1494.398	1491.782	1405.728	1405.967
		3630.217	3630.976	2690.818	2691.277
		3683.373	3684.086		

Table 4: Vibrational frequency (cm⁻¹) of selected geometry-optimized molecules calculated with both uncorrected and DCACP-augmented BLYP functionals.

	$\mu_{\text{H}_2\text{CO}}$	α_{Ar}	$\alpha_{\text{Ar-N}_2}$	Q_{CO_2}	Q_{N_2}	$Q_{\text{C}_6\text{H}_6}$
BLYP	2.295	12.24	24.43	-3.21	-1.13	-5.38
BLYP*	2.294	12.24	24.43	-3.21	-1.13	-5.39

$\alpha_{\text{Ar-N}_2} = \alpha_{zz}^{\text{Ar-N}_2\text{T}}$, $Q = \langle z^2 - \frac{1}{2}x^2 - \frac{1}{2}y^2 \rangle$

Table 5: Polarizabilities, quadrupole, and dipole moments calculated with the uncorrected (BLYP) and DCACP-augmented BLYP (BLYP*) functionals. All values are in atomic units, except for dipole moments which are quoted in debye.

	cutoff [Ry]	E_{\min} [kcal/mol]	r_{\min} [Å]
SG	150	-0.20	3.85
TM	70	-0.20	3.80
TM*	70	-0.20	3.80
VDB	40	-0.20	3.80

Table 6: A comparative study on DCACPs applied in conjunction with various pseudopotential types: Goedecker *et al.* (SG), Troullier-Martins (TM), and Vanderbilt (VDB). N₂ dimer calculated with the DCACP-augmented PBE functional is used for illustration. TM* represents the one which includes DCACP as the f channel in the Troullier-Martins pseudopotential.