

NOF theory as an alternative to DFT

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Outline

- 1 Introduction to the Natural Orbital Functional Theory (NOFT)
- 2 The intrapair electron correlation
 - an independent pair model: PNOF5
- 3 The interpair electron correlation
 - an interacting pair model: PNOF6
- 4 Closing Remarks

The exact energy functional

Consider an N-electron molecule described by a non-degenerate state Ψ .

\hat{H} has only one- and two-particle operators, so the electronic energy in the BO approximation is an explicitly known functional of the spinless 1- and 2-RDMs:

$$E[N, \Gamma, D] = -\frac{1}{2} \int \nabla_1^2 \Gamma(\mathbf{r}'_1, \mathbf{r}_1) |_{\mathbf{r}'_1=\mathbf{r}_1} d\mathbf{r}_1 + \int \Gamma(\mathbf{r}_1, \mathbf{r}_1) v(\mathbf{r}_1) d\mathbf{r}_1 \\ + \int \frac{D(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_1, \mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_1 d\mathbf{r}_2$$

$$\Gamma(\mathbf{r}'_1, \mathbf{r}_1) = N \sum_{\sigma_1} \int \Psi^*(\mathbf{r}'_1, \sigma_1, \mathbf{x}_2, \dots, \mathbf{x}_N) \Psi(\mathbf{r}_1, \sigma_1, \mathbf{x}_2, \dots, \mathbf{x}_N) d\mathbf{x}_2 \dots d\mathbf{x}_N$$

$$D(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_1, \mathbf{r}_2) = \frac{N(N-1)}{2} \sum_{\sigma_1, \sigma_2} \int |\Psi(\mathbf{r}_1, \sigma_1, \mathbf{r}_2, \sigma_2, \mathbf{x}_3, \dots, \mathbf{x}_N)|^2 d\mathbf{x}_3 \dots d\mathbf{x}_N$$

$$\Gamma(\mathbf{x}'_1, \mathbf{x}_1) = \frac{2}{N-1} \int D(\mathbf{x}'_1, \mathbf{x}_2; \mathbf{x}_1, \mathbf{x}_2) d\mathbf{x}_2 \quad \Rightarrow \quad E[N, \Gamma, D] = E[N, D]$$

The variational approach in quantum chemistry

- The wavefunction theories (CI, CC, ...)

- Fundamental Variable: $\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N) \Rightarrow D_\Psi$ (by contraction)

- The ground-state energy: $E_0 = \inf_{\Psi \in \mathcal{L}_N} E[\Psi] = E[\Psi_0] \equiv E[N, D_{\Psi_0}]$

- The variational theories without wavefunction

Method :	DFT	1DMFT		2DMFT
Variable :	$\rho_\Psi(\mathbf{r})$	$\Gamma_\Psi(\mathbf{x}'_1, \mathbf{x}_1)$		$D_\Psi(\mathbf{x}'_1, \mathbf{x}'_2; \mathbf{x}_1, \mathbf{x}_2)$
			(reconstruction)	
Functional :	$E_\Psi[N, \rho_\Psi]$	$E_\Psi[N, \Gamma_\Psi]$	\implies	$E[N, D_\Psi]$
	(HK)	(Gilbert)		(exact)

The N-representability Problem in DFT and 1DMT

- ① The N-representability of $\rho(\Gamma)$: $\rho_{\Psi}(\Gamma_{\Psi}), \Psi \Leftrightarrow \rho(\Gamma)$

- the necessary and sufficient conditions are known

- DFT: $\rho \geq 0, \int \rho(\mathbf{r}) d\mathbf{r} = N$
- 1DMFT: $0 \leq \Gamma \leq ql, \text{Tr}(\Gamma) = N$

- ② The functional N-representability: $E_{\Psi}[N, \rho_{\Psi}] (E_{\Psi}[N, \Gamma_{\Psi}])$

$$E[\Psi] = E[D_{\Psi}] \Leftrightarrow E[\rho_{\Psi}] (E[\Gamma_{\Psi}])$$

- some practical necessary conditions known for the 2-RDM

$$D \geq 0, Q \geq 0, G \geq 0$$

Natural Orbitals and Occupation Numbers

The 1-RDM can be diagonalized by a unitary transformation of the spin-orbitals $\{\phi_i(\mathbf{x})\}$:

$$\Gamma_{ki} = n_i \delta_{ki}, \quad \Gamma(\mathbf{x}'_1, \mathbf{x}_1) = \sum_i n_i \phi_i(\mathbf{x}'_1) \phi_i^*(\mathbf{x}_1)$$

$\phi_i(\mathbf{x})$: natural spin-orbital

n_i : occupation number

- $E_\Psi[N, \Gamma_\Psi] \Rightarrow E_\Psi[N, \{n_i, \phi_i\}]$
- necessary and sufficient conditions for N-representability of Γ :

$$0 \leq n_i \leq 1, \quad \sum_i n_i = N$$

The electronic energy in NOFT

The energy $E[N, \Gamma, D]$ is expressed in terms of the diagonal 1-RDM:

$$E[N, \{n_i, \phi_i\}] = \sum_i n_i \mathcal{H}_{ii} + \sum_{ijkl} D[n_i, n_j, n_k, n_l] \langle kl | ij \rangle$$

- \mathcal{H}_{ii} : core-Hamiltonian
- $\{n_i\}$: occupation numbers
- $\langle kl | ij \rangle$: 2e- integrals
- $\{\phi_i(\mathbf{x})\}$: natural orbitals

2-RDM: $D[n_i, n_j, n_k, n_l] \Leftarrow$ reconstruction functional

Advantage of NOFT with respect to DFT

the kinetic energy is explicitly defined and
does not require the construction of a functional

1. introduction to the NOF theory
2. the intrapair electron correlation
3. the interpair electron correlation

the energy functionals, the N-representability,
 the natural orbital functional
 the reconstruction functional (bottom-up method)

Cumulant expansion of the 2-RDM

$$D_{pq,rt}^{\sigma\sigma,\sigma\sigma} = \frac{n_p^\sigma n_q^\sigma}{2} (\delta_{pr}\delta_{qt} - \delta_{pt}\delta_{qr}) + \lambda_{pq,rt}^{\sigma\sigma,\sigma\sigma} \quad (\sigma = \alpha, \beta)$$

$$D_{pq,rt}^{\alpha\beta,\alpha\beta} = \frac{n_p^\alpha n_q^\beta}{2} \delta_{pr}\delta_{qt} + \lambda_{pq,rt}^{\alpha\beta,\alpha\beta}$$

$$\lambda_{pq,rt}^{\sigma\sigma,\sigma\sigma} = -\frac{\Delta_{pq}^{\sigma\sigma}}{2} (\delta_{pr}\delta_{qt} - \delta_{pt}\delta_{qr}) \quad , \quad \lambda_{pq,rt}^{\alpha\beta,\alpha\beta} = -\frac{\Delta_{pq}^{\alpha\beta}}{2} \delta_{pr}\delta_{qt} + \frac{\Pi_{pr}}{2} \delta_{pq}\delta_{rt}$$

Int. J. Quantum Chem. 106, 1093 (2006)

Δ : real symmetric matrix ($\Delta_{pq}^{\sigma_1\sigma_2} = \Delta_{qp}^{\sigma_2\sigma_1}$)

Sum Rules: $\sum_{q \neq p} \Delta_{pq}^{\sigma\sigma} = n_p^\sigma (1 - n_p^\sigma)$, $\sum_q \Delta_{pq}^{\alpha\beta} = \Pi_{pp}$

Π : spin-independent Hermitian matrix

($\Pi_{pr}^{\alpha\alpha} = \Pi_{pr}^{\alpha\beta} = \Pi_{pr}^{\beta\alpha} = \Pi_{pr}^{\beta\beta} = \Pi_{pr}$, $\Pi_{pr} = \Pi_{rp}^*$)

Singlets: $|SM_S\rangle = |00\rangle$

1 spin-restricted formalism:

- $|\phi_i\rangle = |\varphi_p\rangle \otimes |\sigma\rangle$, $\varphi_p(\mathbf{r}) = \varphi_p^\alpha(\mathbf{r}) = \varphi_p^\beta(\mathbf{r})$

- $n_p^\alpha = n_p^\beta = n_p$, $2 \sum_p n_p = N$

- $\Delta_{pq}^{\alpha\alpha} = \Delta_{pq}^{\alpha\beta} = \Delta_{pq}^{\beta\alpha} = \Delta_{pq}^{\beta\beta} = \Delta_{pq}$

2 $\langle \widehat{S}^2 \rangle = 0 \Rightarrow \Delta_{pp} = n_p^2$, $\Pi_{pp} = n_p$ (J. Chem. Phys. 131, 021102, 2009).

$$\Delta_{pq} = n_p^2 \delta_{pq} + \Delta(n_p, n_q)(1 - \delta_{pq}), \quad \sum_q \Delta_{pq} = n_p$$

$$\Pi_{pq} = n_p \delta_{pq} + \Pi(n_p, n_q)(1 - \delta_{pq})$$

The N-representability and off-diagonal elements

- 1 Analytic constraints imposed by necessary positivity conditions of the 2-matrix N-representability

- $D \geq 0, Q \geq 0$

$$\Delta(n_p, n_q) \leq n_p n_q, \quad \Delta(n_p, n_q) \leq h_p h_q \quad (h_p = 1 - n_p)$$

- $G \geq 0$

$$\Pi^2(n_p, n_q) \leq [n_p h_q + \Delta(n_p, n_q)] [h_p n_q + \Delta(n_p, n_q)]$$

- 2 PNOF:

$$E = \sum_p n_p (2\mathcal{H}_{pp} + \mathcal{J}_{pp}) + \sum'_{pq} [n_q n_p - \Delta(n_q, n_p)] (2\mathcal{J}_{pq} - \mathcal{K}_{pq}) + \sum'_{pq} \Pi(n_q, n_p) \mathcal{L}_{pq}$$

Implemented Approximations

- PNOF1: Int. J. Quan. Chem. 106, 1093, 2006
- PNOF2: J. Chem. Phys. 126, 214103, 2007
- PNOF3: J. Chem. Phys. 132, 031103, 2010
- PNOF4: J. Chem. Phys. 133, 111101, 2010
- **PNOF5** (n_c)
 - $n_c=1$: PNOF5, J. Chem. Phys. 134, 164102, 2011
 - $n_c>1$: PNOF5e, J. Chem. Phys. 139, 234109, 2013
- **PNOF6**: J. Chem. Phys. 141, 044107, 2014

strengths and weaknesses: Int. J. Quantum Chem. 113, 620, 2013

Off-diagonal elements of Δ - and Π -matrices ($p \neq q$)

PNOF5 (n_c): $g = 1, \dots, F$ ($F = N/2$)

$$\Delta^g(n_p, n_q) = n_p n_q \delta_{p\Omega_g} \delta_{q\Omega_g}, \quad \delta_{p\Omega_g} = \begin{cases} 1, & p \in \Omega_g \\ 0, & p \notin \Omega_g \end{cases}$$

$$\Pi^g(n_p, n_q) = \delta_{p\Omega_g} \delta_{q\Omega_g} \begin{cases} -\sqrt{n_p n_q}, & p=g \text{ or } q=g \\ \sqrt{n_p n_q}, & p, q > F \end{cases}$$

- Ω_g is a subspace containing an orbital g below the Fermi level ($g \leq F$), and n_c orbitals with $p > F$. [PNOF5: $\Omega_g \equiv (g, \tilde{g})$]
- sum rule: $\sum_{q \in \Omega_g} n_q = 1$ ($g = 1, \dots, F$) [PNOF5: $n_g + n_{\tilde{g}} = 1$]
- subspaces are mutually disjoint: $\Omega_{g1} \cap \Omega_{g2} = \emptyset$

note: If $(p \in \Omega_{g1}) \cap (q \in \Omega_{g2}) \rightarrow \Delta, \Pi = 0 \rightarrow D^{HF}$

The energy functional for PNOF5e (real orbitals)

$$E = \sum_{g=1}^F E_g + \sum_{f \neq g}^F \sum_{p \in \Omega_f} \sum_{q \in \Omega_g} n_p n_q (2\mathcal{J}_{qp} - \mathcal{K}_{qp})$$

$$E_g = \sum_{p \in \Omega_g} n_p (2\mathcal{H}_{pp} + \mathcal{J}_{pp}) + \sum_{p \neq q} \Pi^g(n_p, n_q) \mathcal{K}_{qp}$$

$$\Pi^g(n_p, n_q) = \delta_{p\Omega_g} \delta_{q\Omega_g} \begin{cases} -\sqrt{n_p n_q}, & p=g \text{ or } q=g \\ \sqrt{n_p n_q}, & p, q > F=N/2 \end{cases}$$

Solution: self-consistent iterative diagonalization procedure

J. Comp. Chem. 30, 2078 (2009)

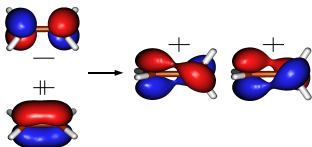
1. introduction to the NOF theory
2. the intrapair electron correlation
3. the interpair electron correlation

the independent pair model: PNOF5 (n_c)

diradicals, homolytic dissociations

A generating wavefunction of PNOF5e (top-down method)

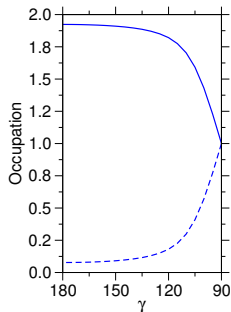
Ethylene Torsion (cc-pVDZ)



Natural Orbital Functional Theory correctly describes degeneracy effects in diradical reactions

	ΔE (kcal/mol)
CASPT2(12,12)	65.5
PNOF5	65.6
B3LYP [‡]	63.8
PBE0 [‡]	60.9
M06-2X [‡]	66.9

[‡] Broken symmetry energies for TS. $\langle S^2 \rangle = 1.01$



J. Chem. Phys. 134, 164102, 2011

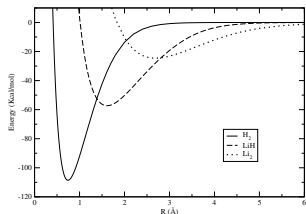
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Dissociation curves for H_2 , LiH and Li_2 (aug-cc-pVTZ)



	PNOF5 ($n_c=1$)		PNOF5e ($n_c>1$)		Exp.	
	R_e	D_e	R_e	D_e	R_e	D_e
H_2	0.756	95.4	0.743	108.6	0.743	109.5
LiH	1.631	44.7	1.613	57.3	1.595	58.0
Li_2	2.703	12.6	2.692	24.6	2.673	24.4

	PNOF5 ($n_c=1$)			PNOF5e ($n_c>1$)			Exp.		
	ω_e	$\omega_e X_e$	$\omega_e Y_e$	ω_e	$\omega_e X_e$	$\omega_e Y_e$	ω_e	$\omega_e X_e$	$\omega_e Y_e$
H_2	4221.7	124.3	0.5	4395.0	121.6	0.8	4401.2	121.3	0.8
LiH	1306.0	24.2	0.2	1382.3	21.7	0.2	1405.5	23.2	0.2
Li_2	354.7	-66.9	-14.4	348.5	3.9	0.1	351.4	2.6	0.0

Errors in total energies (kcal/mol)

	PNOF5 ($n_c=1$)	PNOF5e ($n_c>1$)	CCSD(T)*
H ₂	13.2	0.0	-1.172756
LiH	19.9	2.3	-8.048590
Li ₂	26.7	4.8	-14.954066

* reference values at the equilibrium bond length in Hartrees

aug-cc-pVTZ basis set

The bottom-up and top-down methods

(J. Mod. Phys. 4, 391, 2013)

$$\Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) = \sum C_l(\{n_i\}) \Phi_l(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$$

$$E[\Psi] \equiv E[N, D_\Psi]$$

$$\Downarrow$$

$$E[N, \{n_i, \phi_i\}]$$

$$\Uparrow$$

$$D[n_i, n_j, n_k, n_l]$$

N-representability conditions (D, Q, G, ...)

A generating wavefunction of PNOF5e (APSG)

$$|0\rangle = \prod_{g=1}^F \hat{\psi}_g^\dagger |vac\rangle = \prod_{g=1}^F \left(\sqrt{n_g} \hat{a}_g^\dagger \hat{a}_{\bar{g}}^\dagger - \sum_{p \in \Omega'_g} \sqrt{n_p} \hat{a}_p^\dagger \hat{a}_{\bar{p}}^\dagger \right) |vac\rangle$$

$$\sum_{p \in \Omega_g} n_p = 1, \quad \Omega_{g1} \cap \Omega_{g2} = \emptyset$$

$$E^{exact} \leq E^{APSG} [\{c_p\}, \{\varphi_p\}] \leq E^{PNOF5e} [\{n_p\}, \{\varphi_p\}]$$

$$\text{PNOF5: } |0\rangle = \prod_{g=1}^F \left(\sqrt{n_g} \hat{a}_g^\dagger \hat{a}_{\bar{g}}^\dagger - \sqrt{n_{g'}} \hat{a}_{g'}^\dagger \hat{a}_{\bar{g}'}^\dagger \right) |vac\rangle \quad (\text{GVB-PP})$$

(Pernal, Comput. Theor. Chem. 1003, 127, 2013; Piris, J. Chem. Phys. 139, 064111, 2013)

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diradicals, homolytic dissociations

A generating wavefunction of PNOF5e (top-down method)

APSG generating wavefunction of PNOF5e

$$|0\rangle = |\Phi_0\rangle + |\Phi_d\rangle + |\Phi_q\rangle + \dots + |\Phi_F\rangle, \quad F = N/2$$

$$|\Phi_0\rangle = d_0 |\Psi_{HF}\rangle \qquad |\Phi_d\rangle = -\sum_{g=1}^F \sum_{p \in \Omega'_g} d_g^p |\Psi_{g\bar{g}}^{p\bar{p}}\rangle$$

$$|\Phi_q\rangle = \sum_{g < f}^F \sum_{p \in \Omega'_g} \sum_{q \in \Omega'_f} d_{gf}^{pq} |\Psi_{g\bar{g}f\bar{f}}^{p\bar{p}q\bar{q}}\rangle$$

...

$$|\Phi_{N/2}\rangle = (-1)^F \sum_{p \in \Omega'_1} \sum_{q \in \Omega'_2} \dots \sum_{r \in \Omega'_F} d_{12\dots F}^{pq\dots r} |\Psi_{1\bar{1}2\bar{2}\dots F\bar{F}}^{p\bar{p}q\bar{q}\dots r\bar{r}}\rangle$$

$$d_0 = \sqrt{n_1 n_2 \dots n_F}, \quad d_g^p = d_0 \sqrt{\frac{n_p}{n_g}}, \quad d_{gf}^{pq} = d_0 \sqrt{\frac{n_p n_q}{n_g n_f}}, \quad \dots$$

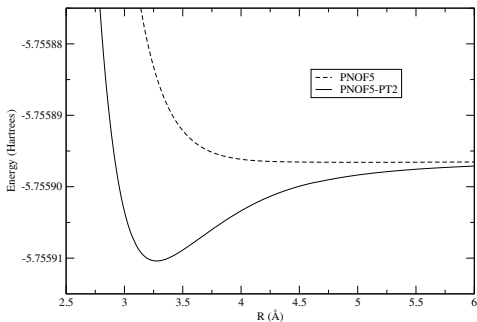
PNOF5-PT2

- The resulting work formulas involve only matrix elements between pure determinants like occurs in the standard single-reference perturbation theory. One needs to consider only $\{|\Psi_a^s\rangle\}$ and $\{|\Psi_{ab}^{su}\rangle\}$ excited determinants.
- No need to solve a system of linear equations for the corrections. The size-consistency is ensured.
- perturbative corrections to $|0\rangle$:

$$E^{(2)} = - \sum_{K=1}^M \frac{\langle \tilde{0} | \hat{V} | K \rangle \langle \tilde{K} | \hat{V} | 0 \rangle}{E_K - E_0} = E_0^{(2)} + E_d^{(2)} + E_q^{(2)}$$

Dissociation of the helium dimer (aug-cc-pV5Z)

- PNOF5 curve is repulsive (no correlation between pairs)
- PNOF5-PT2: $|\Psi_{p\bar{p}}^{su}\rangle$ are excluded from $E^{(2)}$
- dissociation limit = $2 \times E(\text{He}) \rightarrow$ size-consistency of the method



the interpair electron correlation in NOF theory

*PNOF5-PT2 is not
really a NOF theory*

⇒

*Can we recover the missing
correlation from the outset
introducing interactions
between electron pairs in the
framework of the NOF theory?*

Two challenges:

- 1 accomplish this within the mentioned N -representability constraints.
- 2 restrict ourselves to the world of the JKL -only NOFs, to take advantage of the simplicity of this functional form.

Off-diagonal elements of Δ - and Π -matrices for PNOF6

$$\Delta_{qp} = \begin{cases} e^{-2S} h_q h_p \\ \frac{\gamma_q \gamma_p}{S_\gamma} \\ e^{-2S} n_q n_p \end{cases} \quad \Pi_{qp} = \begin{cases} -e^{-S} (h_q h_p)^{1/2} & q \leq F, p \leq F \\ -\Pi_{qp}^\gamma & q \leq F, p > F \\ -\Pi_{qp}^\gamma & q > F, p \leq F \\ e^{-S} (n_q n_p)^{1/2} & q > F, p > F \end{cases}$$

$$S = \sum_1^F h_q = \sum_{F+1}^N n_q, \quad S_\gamma = \sum_{q=1}^F \gamma_q = \sum_{q=F+1}^N \gamma_q, \quad S_\alpha = \sum_{q=1}^F \alpha_q = \sum_{q=F+1}^N \alpha_q$$

$$\gamma_p = n_p h_p + \alpha_p^2 - \alpha_p S_\alpha, \quad \alpha_p = \begin{cases} e^{-S} h_p, & 1 \leq p \leq F \\ e^{-S} n_p, & F < p \leq N \end{cases}$$

$$\Pi_{qp}^\gamma = \left(n_q h_p + \frac{\gamma_q \gamma_p}{S_\gamma} \right)^{1/2} \left(h_q n_p + \frac{\gamma_q \gamma_p}{S_\gamma} \right)^{1/2}$$

PNOF6: A natural orbital JKL-functional

$$E = \sum_{g=1}^F E_g + \sum_{f \neq g}^F (E_{fg}^{in} + E_{fg}^{out}) + 2 \sum_{p=F+1}^N \sum_{q=1, \neq \tilde{p}}^F E_{pq}^{\gamma}$$

$$E_g = \sum_{p \in \Omega_g} n_p (2\mathcal{H}_{pp} + \mathcal{J}_{pp}) + 2E_{g\tilde{g}}^{\gamma}$$

$$E_{fg}^{in} = (n_f n_g - e^{-2S} h_f h_g) (2\mathcal{J}_{gf} - \mathcal{K}_{gf}) - e^{-S} \sqrt{h_f h_g} \mathcal{L}_{gf}$$

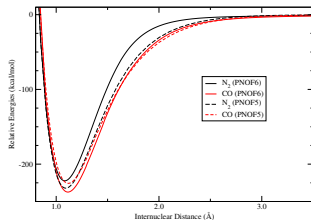
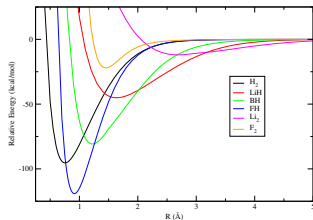
$$E_{fg}^{out} = (1 - e^{-2S}) n_{\tilde{f}} n_{\tilde{g}} (2\mathcal{J}_{\tilde{g}\tilde{f}} - \mathcal{K}_{\tilde{g}\tilde{f}}) + e^{-S} \sqrt{n_{\tilde{f}} n_{\tilde{g}}} \mathcal{L}_{\tilde{g}\tilde{f}}$$

$$E_{pq}^{\gamma} = \left(n_q n_p - \frac{\gamma_q \gamma_p}{S_{\gamma}} \right) (2\mathcal{J}_{pq} - \mathcal{K}_{pq}) - \Pi_{qp}^{\gamma} \mathcal{L}_{pq}$$

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PNOF5-PT2, Dissociation of the Helium Dimer.
 PNOF6, Homolytic dissociations.
 Electron Delocalization, Benzene.

Homolytic dissociations (cc-pVTZ)

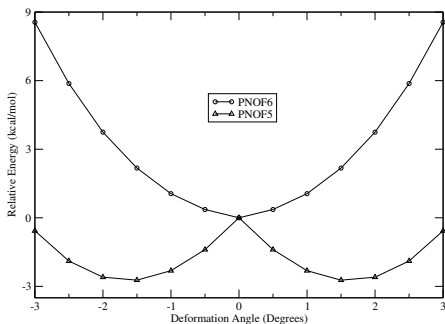


	PNOF5			PNOF6			Experimental		
	R_e	μ	D_e	R_e	μ	D_e	R_e	μ	D_e
H ₂	0.755	0.00	95.3	0.755	0.00	95.3	0.741	0.00	109.5
LiH	1.632	5.75	44.6	1.635	5.72	45.1	1.596	5.88	58.0
BH	1.248	1.50	75.7	1.224	1.43	80.8	1.232	1.27	81.5
FH	0.915	1.87	114.5	0.914	1.80	119.1	0.917	1.82	141.1
F ₂	1.480	0.00	14.1	1.455	0.00	22.0	1.412	0.00	39.2
N ₂	1.090	0.00	239.3	1.084	0.00	222.3	1.098	0.00	228.3
CO	1.116	0.22	225.6	1.114	0.10	237.4	1.128	0.11	259.3

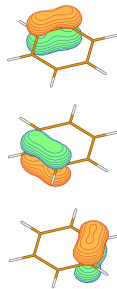
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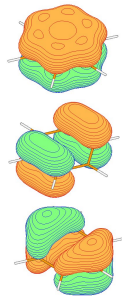
Potential energy curve for the distortion of benzene



PNOF5



PNOF6



The three bonding π orbitals

Closing remarks

- Two natural orbital functionals have been analyzed:
PNOF5: Independent pairs PNOF6: Interacting pairs
- PNOF5 has been obtained by
 - 1 the bottom-up method: cumulant expansion imposing necessary N-representability conditions on 2-RDM
 - 2 the top-down method: a generating wavefunction of APSG type with expansion coefficients expressed by the ONs
- the interactions between pairs can be attained by SC2-MCPT with PNOF5 as a reference: PNOF5-PT2
- The new functional PNOF6 describes the static (non-dynamic) and dynamic correlations in a balanced way.

Acknowledgements

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Thank you for your attention !!!