

Second-order perturbative corrections in NOF theory

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Outline

- 1 The Natural Orbital Functional PNOF5 (JCP 134, 164102, 2011)
 - generating APSG wavefunction \rightarrow top-down method
- 2 PNOF5-PT2 (JCP 139, 064111, 2013; J. Mol. Phys. 2013)
 - Introduction to the SC2-MCPT (JCP 122, 114104, 2005)
 - Examples: He₂, HF, CO, N₂, H-bonds, Isogyric reactions
- 3 Closing Remarks

The electronic energy E for N -electron systems

In NOFT, the energy 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

1-RDM: $\Gamma_{ki} = n_i \delta_{ki}$, $\Gamma(\mathbf{x}'_1 | \mathbf{x}_1) = \sum_i n_i \phi_i(\mathbf{x}'_1) \phi_i^*(\mathbf{x}_1)$

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

The bottom-up and top-down methods

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

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

N -particle energy functional $E[\Psi_N]$

$$\Downarrow$$

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

$$\Uparrow$$

$$\mathbf{D}[\Gamma] = \mathbf{D}[\{n_i\}]$$

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

Antisymmetrized Product of Strongly orthogonal Geminals

- PNOF5 $\Leftrightarrow E(\Psi^{APSG}, 2 \text{ conf, fixed signs for } \{c_p\}) \equiv E(\Psi^{GVB, PP})$

$$E^{exact} \leq E^{APSG} [\{c_p\}, \{\varphi_p\}] \leq E^{PNOF5} [\{n_p\}, \{\varphi_p\}]$$

(Pernal, Comput. Theor. Chem. 1003, 127, 2013)

- A generating wavefunction of PNOF5:

$$|0\rangle = \prod_{g=1}^{N/2} \hat{\psi}_g^\dagger |vac\rangle = \prod_{g=1}^{N/2} \left(\sqrt{n_g} \hat{a}_g^\dagger \hat{a}_g^\dagger - \sqrt{n_{g'}} \hat{a}_g^\dagger \hat{a}_{g'}^\dagger \right) |vac\rangle$$

$$|0\rangle = d_0 |\Psi_{HF}\rangle + \sum_{p=1}^{N/2} d_p \left| \Psi_{p \bar{p}}^{p' \bar{p}'} \right\rangle + \sum_{p < q}^{N/2} d_{pq} \left| \Psi_{p \bar{p} q \bar{q}}^{p' \bar{p}' q' \bar{q}'} \right\rangle + \dots$$

(JCP 139, 064111, 2013)

APSG generating wavefunction of PNOF5

$$|0\rangle = |\Phi_0\rangle + |\Phi_d\rangle + |\Phi_q\rangle + \dots + |\Phi_{N/2}\rangle$$

where

$$|\Phi_0\rangle = d_0 |\Psi_{HF}\rangle$$

$$|\Phi_d\rangle = \sum_{p=1}^{N/2} d_p |\Psi_{p\bar{p}}^{p'\bar{p}'}\rangle$$

$$|\Phi_q\rangle = \sum_{p < q}^{N/2} d_{pq} |\Psi_{p\bar{p}q\bar{q}}^{p'\bar{p}'q'\bar{q}'}\rangle$$

...

$$|\Phi_{N/2}\rangle = d_{12\dots N/2} |\Psi_{1\bar{1}2\bar{2}\dots N/2\bar{N/2}}^{1'\bar{1}'2'\bar{2}'\dots N/2'\bar{N/2}'}\rangle$$

$$d_0 = \sqrt{n_1 n_2 \dots n_{N/2}}, \quad d_p = -d_0 \sqrt{\frac{n_{p'}}{n_p}}, \quad d_{pq} = d_0 \sqrt{\frac{n_{p'} n_{q'}}{n_p n_q}}, \dots$$

spin-parallel and spin-opposite components of the 2-RDM

$$D_{pq,rt} = \frac{n_p n_q}{2} (\delta_{pr} \delta_{qt} - \delta_{pt} \delta_{qr}) (1 - \delta_{qp}) (1 - \delta_{qp'})$$

$$D_{p\bar{q},r\bar{t}} = \frac{n_p n_q}{2} \delta_{pr} \delta_{qt} (1 - \delta_{qp}) (1 - \delta_{qp'}) \\ + \left(\frac{n_p}{2} \delta_{rp} - \frac{\sqrt{n_p n_{p'}}}{2} \delta_{rp'} \right) \delta_{pq} \delta_{rt}$$

PNOF5:

$$E = \sum_{p=1}^N [n_p (2\mathcal{H}_{pp} + \mathcal{J}_{pp}) - \sqrt{n_{p'} n_p} \mathcal{K}_{pp'}] \\ + \sum_{p,q=1}^N " n_q n_p (2\mathcal{J}_{pq} - \mathcal{K}_{pq})$$

Examples of strongly correlated systems

1 diradicals and diradicaloids

- J. Chem. Phys. 134, 164102, 2011
- Chem Phys Chem 12, 1673, 2011

2 homolytic dissociation

- Phys. Chem. Chem. Phys. 13, 20129, 2011
- J. Chem. Theory Comp. 8, 2646, 2012
- TMs (Cr_2), Phys. Chem. Chem. Phys. 15, 2055, 2013

3 IPs by the extended Koopmans' theorem

- J. Chem. Phys. 136, 174116, 2012

4 PNOF5 natural and canonical orbitals

- Chem. Phys. Lett. 531, 272, 2012
- Chem Phys Chem 13, 2297, 2012
- Theor. Chem. Acc. 132, 1298, 2013
- J. Chem. Phys. 138, 151102, 2013

The reciprocal space in the MCPT

MCPT:

- $|0\rangle$: the zero-order ground state
- one seeks perturbative corrections to $|0\rangle$
- overlapping basis in the full M-dimensional space

$$|K\rangle = \begin{cases} |0\rangle, & K = 0 \\ |\Psi_K\rangle, & K \neq 0 \end{cases}$$

$|\Psi_K\rangle$: excited determinants with respect to $|\Psi_{HF}\rangle$

- reciprocal (biorthogonal) vectors

$$\langle \tilde{K} | = \begin{cases} d_0^{-1} \langle \Psi_{HF} |, & K = 0 \\ \langle \Psi_K | - d_K \langle \tilde{0} |, & K \neq 0 \end{cases}$$

$$\langle \tilde{K} | L \rangle = \delta_{KL}$$

Z. Rolik, et. al., J. Chem. Phys. 119, 1922 (2003).

Non-Hermitian zero-order Hamiltonian

- Spectral resolution:

$$\hat{H}^0 = \sum_{K=0}^M E_K |K\rangle \langle \tilde{K}|$$

- $\{|K\rangle\}$ are right and $\{\langle \tilde{K}|\}$ are left eigenvectors of \hat{H}^0
 - E_K -s are free parameters, define the partitioning
 - size-consistency is ensured by omitting projectors
- E_0 is conveniently taken as the zero-order ground state energy:

$$E_0 = E^{(0)} = \langle \tilde{0} | \hat{H} | 0 \rangle = \tilde{E}_{HF} + \tilde{E}_{corr}$$

$$\tilde{E}_{HF} = \langle \Psi_{HF} | \hat{H} | \Psi_{HF} \rangle, \quad \tilde{E}_{corr} = - \sum_{p=1}^{N/2} \sqrt{\frac{n_{p'}}{n_p}} \mathcal{K}_{pp'}$$

The Davidson-Kapuy Partitioning: SC2-MCPT.

- The zero-order excited energies: $E_K = E_0 + \Delta_K$

$$\Delta_K = \begin{cases} \varepsilon_s - \varepsilon_a & a \leq N ; s > N \\ \varepsilon_s + \varepsilon_u - \varepsilon_a - \varepsilon_b & a, b \leq N ; s, u > N \\ \dots & \dots \end{cases}$$

Δ_K : differences between diagonal elements of Fock operator

$$\varepsilon_i = h_{ii} + \sum_{q=1}^{N/2} [2 \langle iq | iq \rangle - \langle iq | qi \rangle]$$

size-consistency is ensured by considering energy denominators as differences of one-particle energies

A. Szabados, et. al., J. Chem. Phys. 122, 114104 (2005).

Lowest order energy corrections

$$E^{(1)} = \langle \tilde{0} | \hat{V} | 0 \rangle = 0, \quad \hat{V} = \hat{H} - \hat{H}^0$$

$$\begin{aligned} E^{(2)} &= - \sum_{K=1}^M \frac{\langle \tilde{0} | \hat{V} | K \rangle \langle \tilde{K} | \hat{V} | 0 \rangle}{E_K - E_0} = - \sum_{K=1}^M \frac{\langle \tilde{0} | \hat{H} | K \rangle \langle \tilde{K} | \hat{H} | 0 \rangle}{\Delta_K} \\ &= \sum_{K=1}^M \frac{\langle \Psi_{HF} | \hat{H} | K \rangle [d_K E^{(0)} - \langle K | \hat{H} | 0 \rangle]}{d_0 \Delta_K} \end{aligned}$$

- non-invariance with respect to the choice of the Fermi vacuum
- one needs to consider only $\{|\Psi_a^s\rangle\}$ and $\{|\Psi_{ab}^{su}\rangle\}$ excited det.

Second-order energy correction

$$E^{(2)} = E_0^{(2)} + E_d^{(2)} + E_q^{(2)}$$

where

$$E_0^{(2)} = 2 \sum_{pr}^{N/2} \frac{|f_{pr}|^2}{\varepsilon_p - \varepsilon_r} + \sum_{pqrt}^{N/2} \frac{\langle pq | rt \rangle [2 \langle rt | pq \rangle - \langle rt | qp \rangle]}{\varepsilon_p + \varepsilon_q - \varepsilon_r - \varepsilon_t}$$

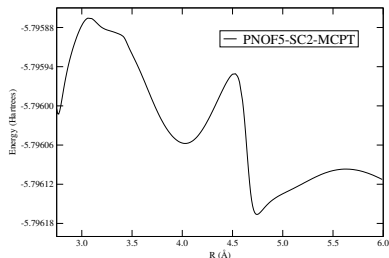
$$E_q^{(2)} = \sum_p^{N/2} \binom{n_{p'}}{n_p} \frac{|\mathcal{K}_{pp'}|^2}{(\varepsilon_{p'} - \varepsilon_p)} + \sum_{pq}^{N/2} \sqrt{\frac{n_{p'} n_{q'}}{n_p n_q}} \frac{[2 \langle pq | p'q' \rangle - \langle pq | q'p' \rangle]^2}{\varepsilon_p + \varepsilon_q - \varepsilon_{p'} - \varepsilon_{q'}}$$

Second-order energy correction

$$\begin{aligned}
 E_d^{(2)} = & 2 \sum_p^{N/2} \sqrt{\frac{n_{p'}}{n_p}} \frac{|f_{pp'}|^2}{(\epsilon_{p'} - \epsilon_p)} + 2 \sum_{pqr}^{N/2} \sqrt{\frac{n_r}{n_{r'}}} \frac{\langle pq | rr \rangle \langle r' r' | pq \rangle}{2\epsilon_r - \epsilon_p - \epsilon_q} \\
 & + 2 \sum_{pr}^{N/2} \frac{f_{rp}}{\epsilon_r - \epsilon_p} \left[\sqrt{\frac{n_{p'}}{n_p}} \langle pr | p' p' \rangle - \sqrt{\frac{n_r}{n_{r'}}} \langle r' r' | pr \rangle \right] \\
 & + 2 \sum_p^{N/2} \sqrt{\frac{n_{p'}}{n_p}} \left\{ \sum_r^{N/2} \frac{f_{rp'} \langle pp | p' r \rangle}{\epsilon_r + \epsilon_{p'} - 2\epsilon_p} + \sum_q^{N/2} \frac{f_{qp} \langle pq | p' p' \rangle}{\epsilon_p + \epsilon_q - 2\epsilon_{p'}} \right. \\
 & + \frac{1}{2} \sum_{rs}^{N/2} \frac{\langle pp | rs \rangle \langle rs | p' p' \rangle}{\epsilon_r + \epsilon_s - 2\epsilon_p} + \sum_{qr}^{N/2} \frac{\langle pq | rp' \rangle \langle pr | qp' \rangle}{\epsilon_p + \epsilon_q - \epsilon_r - \epsilon_{p'}} \\
 & \left. + \sum_{qr}^{N/2} \frac{[\langle pq | rp' \rangle + \langle pr | qp' \rangle] \langle pq | p' r \rangle}{\epsilon_p + \epsilon_q - \epsilon_r - \epsilon_{p'}} \right\}
 \end{aligned}$$

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

- typical phenomenon of dispersion interaction ($E_b = 0.021$ kcal/mol)
- electron correlation effect is almost entirely atomic intrapair
- the interpair correlation should be mostly dispersion type



Note: excitations $|\Psi_{p\bar{p}}^{su}\rangle$ are already in $|0\rangle$

full CI calculations (JCP 137, 204117, 2012)

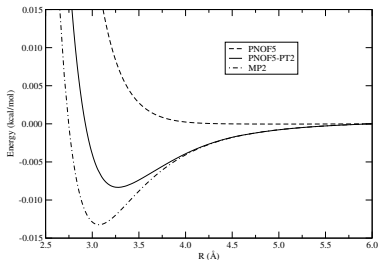
- contribution of $|\Psi_{ab}^{su}\rangle$ with $a \neq b$:
 $2/3 \approx 100\%$ of vdW for same-spin e^-
 $1/3 \rightarrow 50\%$ of vdW for opposite-spin e^-
- contribution of $|\Psi_{p\bar{p}}^{su}\rangle$:
 50% of vdW for opposite-spin e^-

PNOF5-PT2: $|\Psi_{\rho\bar{p}}^{SU}\rangle$ are excluded from $E^{(2)}$

$$\begin{aligned}
 E^{(2)} = & 2 \sum_{pr}^{N/2} \frac{|f_{pr}|^2}{\varepsilon_p - \varepsilon_r} + \sum_{pqrt(q \neq p)}^{N/2} \frac{\langle pq | rt \rangle [2 \langle rt | pq \rangle - \langle rt | qp \rangle]}{\varepsilon_p + \varepsilon_q - \varepsilon_r - \varepsilon_t} \\
 & + 2 \sum_p^{N/2} \sqrt{\frac{n_{p'}}{n_p}} \left[\frac{|f_{pp'}|^2}{(\varepsilon_{p'} - \varepsilon_p)} + \sum_{q(q \neq p)}^{N/2} \frac{f_{qp} \langle pq | p' p' \rangle}{\varepsilon_p + \varepsilon_q - 2\varepsilon_{p'}} \right] \\
 & + 2 \sum_{pr}^{N/2} \frac{f_{rp}}{\varepsilon_r - \varepsilon_p} \left[\sqrt{\frac{n_{p'}}{n_p}} \langle pr | p' p' \rangle - \sqrt{\frac{n_r}{n_{r'}}} \langle r' r' | pr \rangle \right] \\
 & + 2 \sum_{pqr(q \neq p)}^{N/2} \left\{ \sqrt{\frac{n_{p'}}{n_p}} \frac{\langle pq | rp' \rangle \langle pr | qp' \rangle}{\varepsilon_p + \varepsilon_q - \varepsilon_r - \varepsilon_{p'}} + \sqrt{\frac{n_r}{n_{r'}}} \frac{\langle pq | rr \rangle \langle r' r' | pq \rangle}{2\varepsilon_r - \varepsilon_p - \varepsilon_q} \right. \\
 & \quad \left. + \sqrt{\frac{n_{p'}}{n_p}} \frac{[\langle pq | rp' \rangle + \langle pr | qp' \rangle] \langle pq | p' r \rangle}{\varepsilon_p + \varepsilon_q - \varepsilon_r - \varepsilon_{p'}} \right\} \\
 & + \sum_{pq(q \neq p)}^{N/2} \sqrt{\frac{n_{p'} n_{q'}}{n_p n_q}} \frac{[2 \langle pq | p' q' \rangle - \langle pq | q' p' \rangle]^2}{\varepsilon_p + \varepsilon_q - \varepsilon_{p'} - \varepsilon_{q'}}
 \end{aligned}$$

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



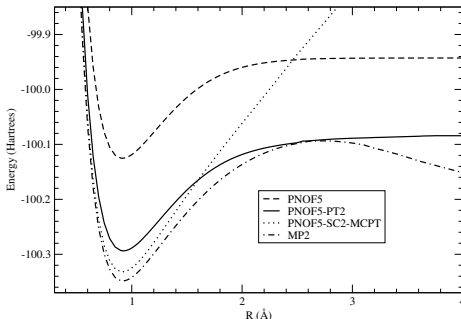
$$E_b = 0.009 \text{ kcal/mol}$$

$$E_b + 1/3 E_b = 0.012 \text{ kcal/mol} \approx E_b^{MP2}$$

\rightarrow Include more orbitals in each geminal:

- better intrapair correlation
- better reference for the PT

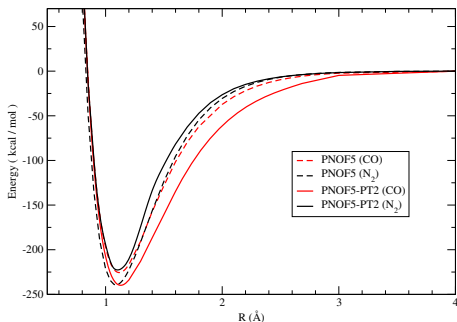
Dissociation curves of the hydrogen fluoride (cc-pVTZ)



	D_e (kcal/mol)
PNOF5	114.5
PNOF5-PT2	134.2
Experiment	141.1

- the excitations between the lowest-weakly and highest-strongly occupied orbitals, which in the limit correspond to the degenerate orbitals, are removed from the whole dissociation process.

Dissociation of the CO and N₂ molecules (cc-pVTZ)



	$D_e(N_2)$	$D_e(CO)$
PNOF5	239.3	225.6
PNOF5-PT2	221.8	238.0
Experiment	225.1	256.2

- PNOF5 shows a wrong order : $D_e(CO) < D_e(N_2)$.
- PNOF5-PT2 recovers the correct order $D_e(N_2) < D_e(CO)$.

(zero-energy has been set at their corresponding energy at 6 Å)

Selected molecular properties: R_e , D_e , ω_e

Mol	PNOF5			PNOF5-PT2			Exp.		
	R_e	ω_e	D_e	R_e	ω_e	D_e	R_{exp}	ω_e	D_e
<i>HF</i>	0.915	4149.3	114.5	0.924	4047.0	134.2	0.917	4138.4	141.1
<i>N₂</i>	1.090	2468.7	239.3	1.103	2326.3	221.8	1.098	2358.6	225.1
<i>CO</i>	1.116	2313.8	225.6	1.129	2199.0	238.0	1.128	2169.8	256.2

- PNOF5 underestimates R_e and overestimates ω_e .
- PNOF5-PT2 increases the predicted equilibrium bond lengths.
- For frequencies, the PNOF5-PT2 values decrease toward the experimental data, particularly, in case of multiple bonds.
- PNOF5-PT2 dissociation energies have improved substantially over the PNOF5 ones, getting closer to the experimental marks.

Errors in binding energies as compared against CCSD(T)

H-bonded DIMER	PNOF5	PNOF5-PT2	PNOF5-SC2-MCPT
(HF) ₂	-2.62	-1.13	-1.02
(H ₂ O) ₂	-2.56	-1.08	-0.76
HF-H ₂ CO	-3.62	-0.01	+2.00
HF-H ₂ O	-3.34	-0.35	+0.80
HCN-H ₃ O ⁺	-6.89	-7.15	-6.38
H ₂ O-H ₃ O ⁺	-10.13	-7.66	-6.58
H ₂ O-OH ⁻	-13.47	-7.95	-6.59
FHF ⁻	-10.56	-8.25	-2.04

- CCSD(T): weakly bonded (HF)₂ → strongly bonded FHF⁻
 (6.70 kcal/mol) → (62.07 kcal/mol)

Errors in reaction energies as compared against CCSD(T)

No	Reaction	PNOF5	PNOF5-PT2	SC2-MCPT	MP2
1	$CH_2(^1A_1) + H_2 \rightarrow CH_4$	19.9	-1.8	-7.5	-7.12
2	$F_2 + H_2 \rightarrow 2HF$	10.8	-6.4	-14.5	-7.6
3	$H_2O_2 + H_2 \rightarrow 2H_2O$	3.1	-2.2	-3.3	-4.1
4	$CO + H_2 \rightarrow H_2CO$	-0.3	2.4	5.8	-0.4
5	$C_2H_2 + H_2 \rightarrow C_2H_4$	0.5	8.0	3.5	2.1
6	$HNO + 2H_2 \rightarrow H_2O + NH_3$	11.8	-1.2	-5.3	-4.5
7	$H_2CO + 2H_2 \rightarrow CH_4 + H_2O$	8.7	1.3	-4.4	-1.3
Mean Absolute Deviation		7.9	3.3	6.3	3.9

- All calculations at the experimental geometries. cc-pVTZ basis set.
- PNOF5 is worse than MP2: lack of dynamical correlation.
- Exception: reactions 4 and 5. Best result is PNOF5.
- H₂: PNOF5 \equiv PNOF5-PT2, SC2-MCPT recovers part of dynamical correlation.
- the double counting of excited determinants is important.

Errors in reaction energies as compared against CCSD(T)

Reaction	PNOF5	PNOF5-PT2	SC2-MCPT	MP2
$N_2 + 3H_2 \rightarrow 2NH_3$	12.1	7.3	4.4	0.5
$CO + 3H_2 \rightarrow CH_4 + H_2O$	8.4	3.7	1.4	-1.7
$HCN + 3H_2 \rightarrow CH_4 + NH_3$	9.0	12.5	3.2	1.2
$C_2H_2 + 3H_2 \rightarrow 2CH_4$	6.5	12.7	-0.6	0.9
Mean Absolute Deviation	9.0	9.0	2.4	1.1

- All calculations at the experimental geometries. cc-pVTZ basis set.
- PNOF5 and PNOF5-PT2 are worse than MP2.
- H₂: PNOF5 \equiv PNOF5-PT2, SC2-MCPT recovers part of dynamical correlation.
- the intrapair electron correlation plays a dominating role with respect to the double counting of excited determinants

Conclusions

- the generating PNOF5-wavefunction is a two-configuration APSG (GVB or PP).
- a computationally tractable second-order perturbation theory PNOF5-PT2 has been derived from the SC2-MCPT. This ansatz involves only double excitations from different spatial orbitals to account for the interpair correlation.
- PNOF5-PT2 is a good choice when the intrapair electron correlation is a minor effect.
- future work: better description of the intrapair electron correlation with an extended version of PNOF5

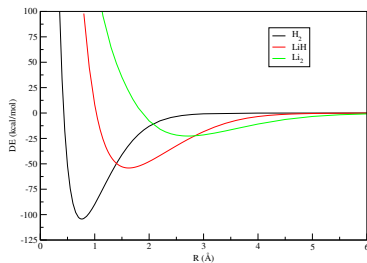
PNOF5e: top-down method

$$|0\rangle = \prod_{g=1}^{N/2} \hat{\psi}_g^\dagger |vac\rangle = \prod_{g=1}^{N/2} \left(\sqrt{n_g} \hat{a}_g^\dagger \hat{a}_g^\dagger - \sum_{p \in \Omega'_g} \sqrt{n_p} \hat{a}_p^\dagger \hat{a}_p^\dagger \right) |vac\rangle$$

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

$$E = 2 \sum_{p=1}^{\infty} n_p \mathcal{H}_{pp} + \sum_{g=1}^{N/2} \left\{ n_g \mathcal{J}_{gg} + \sum_{p,q \in \Omega'_g} \sqrt{n_q n_p} \mathcal{K}_{pq} \right. \\ \left. - 2 \sum_{p \in \Omega'_g} \sqrt{n_g n_p} \mathcal{K}_{pg} \right\} + \sum_{f \neq g}^{N/2} \sum_{p \in \Omega_f} \sum_{q \in \Omega_g} n_q n_p (2\mathcal{J}_{pq} - \mathcal{K}_{pq})$$

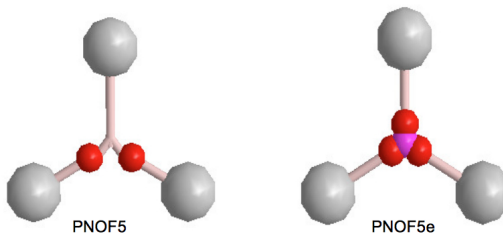
Dissociation curves for H₂, LiH and Li₂



Mol	PNOF5		PNOF5e		Exp.	
	R _e	D _e	R _e	D _e	R _e	D _e
H ₂	0.77	93.4	0.76 (0.74)	104.3 (108.6)	0.74	109.5
LiH	1.64	43.8	1.61 (1.60)	55.0 (57.4)	1.60	58.0
Li ₂	2.71	12.2	2.71 (2.69)	22.6 (24.5)	2.67	24.4

- aug-cc-pVDZ (aug-cc-pVTZ) basis set.

Properties of BCPs and NNM of the H_3^+ cluster



NOF	#	ϵ	Bond Strain
PNOF5	2	3.3104 ± 0.0000	0.2294 ± 0.0000
PNOF5e	3	1.8737 ± 0.0085	0.0000 ± 0.0000

- cc-pVTZ basis set.
- the values of ρ , $\nabla^2\rho$ and energy densities G and H, are similar.

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Thank you for your attention !!!