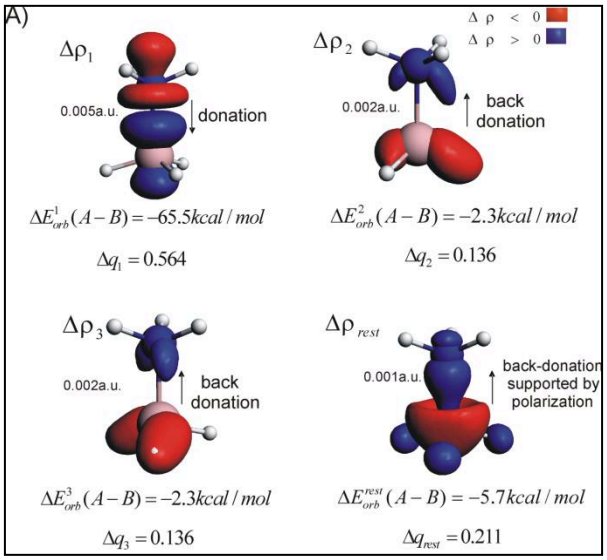
Exercise1. Getting started with the simple bond formed between ammonia and borane – typical *donor–acceptor* bond $H_3N \rightarrow BH_3$.

- Enter the directory /home/baw/baw-workshop/mitoraj/Exercise1 by taping in console : cd /home/baw/baw-workshop/mitoraj/Exercise1
- Then copy the input files to your directory (/home/baw/baw-workshop/uXX) by taping: cp *.in /home/baw/baw-workshop/uXX
- Then go back to your directory by: /home/baw/baw-workshop/uXX
- Run SP calculations for the first fragment by: subadf nh3_frag1.in
- Run SP calculations for the second fragment by: subadf bh3_frag2.in
- Run final calculations by taping: subadf AB-NOCV.in (wait until finished). (please, remember to change the path to *.t21 files /home/baw/baw-workshop/uxx).
- Open the file with the numerical EDA results (AB-NOCV.epa), writh down the results.
- Run adfview to visualize NOCV deformation density by taping: adfview AB-NOCV.t21 &
- From the upper menu click sequentially “Add”→”Isosurface:Double(+/-)”, then change the contour value to 0.005a.u.
- Click the empty bookmark; you should see various grid properties (Deensity, etc.), then click the option “NOCV Def Densities” – it shows NOCV-deformation density contribution ordered by their importance; click the first one; you should see donation from the lone electron pair of ammonia to the empty 2p orbital of boron atom ☺ (red color shows charge outflow, whereas the red charge accumulation due to formation of $NH_3 \rightarrow BH_3$ bonding).
- Open the AB-NOCV.out file and go to section “ETS-NOCV-decomposition”, it is at the end of file. Then take a look that at section ”3. Orbital Interaction Energy Contributions from each NOCV pair (in kcal/mol)”, where the orbital interaction stabilization is printed out (you should see that the first contribution corresponds to -70.25 kcal/mol).
- Fill up the table at the end of this file….:)

Your compiled NOCV based results on $NH_3 \rightarrow BH_3$ should look similarly to this figure:



The numerical values in the above figure and your values from the output file differ because I have used other computational details…☺

Exercise2. Why ammonia (with one lone electron pair) can form the bond with iodine (containing three lone pairs)? It is fully contrary to expectation from VSEPR model (Valence Shell Electron Pair Repulsion). Analysis of *halogen bonding* formed between ammonia and trifluoroiodomethane (CF_3I).

All necessary input files (nh3_frag1.in, icf3_frag2.in, nh3-if3-nocv.in) are in the directory : /home/baw/baw-workshop/mitoraj/Exercise2

Copy them to your directory and repeat the steps as in the previous Exercise 1.

Exercise3. Analysis of carbon–iodine bond in $F_3C–I$ using open shell fragments $F_3C\uparrow + \downarrow I$.

All necessary input files (I_frag1.in, cf3_frag2.in and I-CF3-NOCV.in) are in the directory : /home/baw/baw-workshop/mitoraj/Exercise3. Copy them to your directory and repeat the steps as in the previous Exercise 1.

Important remark! When considering either open shell fragments or open shell molecule one must consider deformation densities stemming from alpha- and beta-deformation matrices. Accordingly, one have in the adfview the NOCV Def Densities from **alpha set** $\Delta\rho_i(\alpha)$ and and **beta set** $\Delta\rho_i(\beta)$ separately. In order to obtain fullpicture of contribution one must accordingly add the right corresponding to each other deformation density channels from the alpha and the beta sets $\Delta\rho_i(\alpha)+\Delta\rho_i(\beta)$ using **"Calculated Field"** option in adfview.

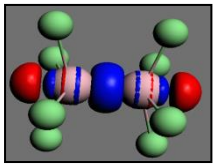
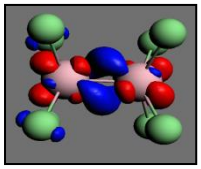
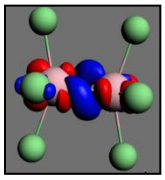
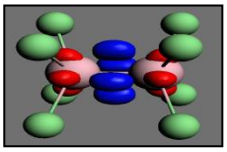
Exercise4. Analysis of carbon–carbon bond in ethane $H_3C\uparrow + \downarrow CH_3$. All necessary input files (ch3_frag1.in, ch3_frag2.in, CH3-CH3-NOCV.in) are in the directory : /home/baw/baw-workshop/mitoraj/Exercise4. Copy them to your directory and repeat the steps as in the previous examples.

Exercise 5. Analysis of C=C bond in ethene $H_2C\uparrow\uparrow+\downarrow\downarrow CH_2$

All necessary input files (ch2_frag1.in, ch2_frag2.in, CH2-CH2-NOCV.in) are in the directory : /home/baw/baw-workshop/mitoraj/Exercise5. Copy them to your directory and repeat the steps as in the previous examples.

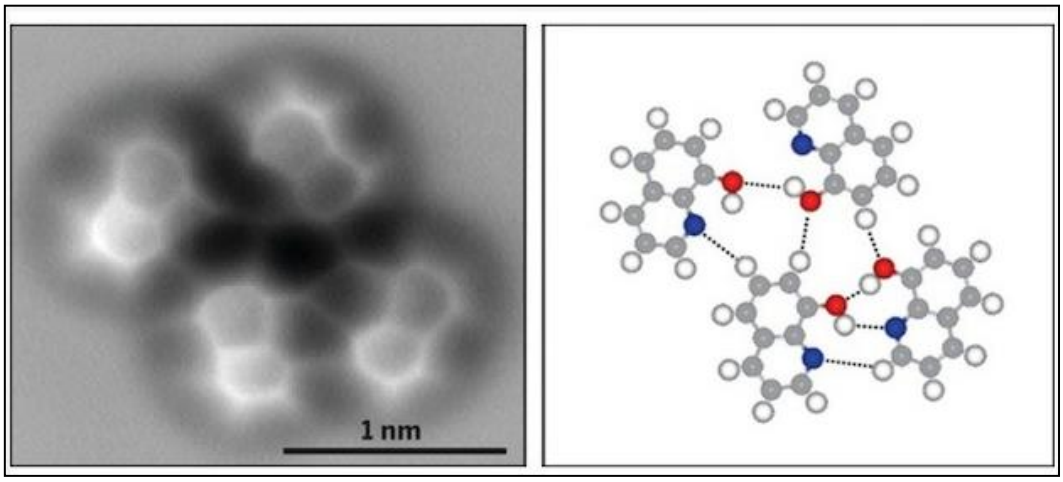
Exercise6. Analysis of quadruple bond between Re atoms in $[Cl_4ReReCl_4]^{2-}$ ($Cl_4Re\uparrow\uparrow\uparrow\uparrow+\downarrow\downarrow\downarrow\downarrow Re\ Cl_4$).

All necessary input files (recl4_frag1.in, recl4_frag2.in, Re-Re-NOCV.in) are in the directory : /home/baw/baw-workshop/mitoraj/Exercise6. Copy them to your directory and repeat the steps as in the previous examples. Finally four (σ, $\pi1$, $\pi2$ and δ) contributions shall be seen:

Exercise7. Analysis of weak homopolar dihydrogen interaction CH···HC formed between closed shell two dodecahedran hydrocarbon units. All necessary input files (frag1.in,frag2.in, CH-HC-NOCV.in) are in the directory : /home/baw/baw-workshop/mitoraj/Exercise7.

Exercise8. Interaction between four monomers of tetra-hydroxoquinoline bonded via O···HO hydrogen bonds. All necessary input files (quin1.in, quin2.in, quin3.in, quin4.in and Quin-tetramer-NOCV.in) are in the directory /home/baw/baw-workshop/mitoraj/Exercise8. Compare the most important NOCV-deformation density channels to the experimental picture of bonding emerging from the tunneling microscope:



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Fill up the table below.

TZ2p+/BP86/kcal/mol	ΔE_{int}	ΔE_{orb}	ΔE_{elstat}	ΔE_{Pauli}	$\Delta E_{dispersion}$
$H_3N \rightarrow BH_3$					
$H_3N \cdots ICF_3$					
$F_3C\uparrow + \downarrow I$					
$H_3C\uparrow + \downarrow CH_3$					
$H_2C\uparrow\uparrow + \downarrow\downarrow CH_2$					
LRe$\uparrow\uparrow\uparrow\uparrow + \downarrow\downarrow\downarrow\downarrow$ReL					
dimer-dodekahedran					