Supporting Information for:

How do electron localization functions describe π-electron delocalization?

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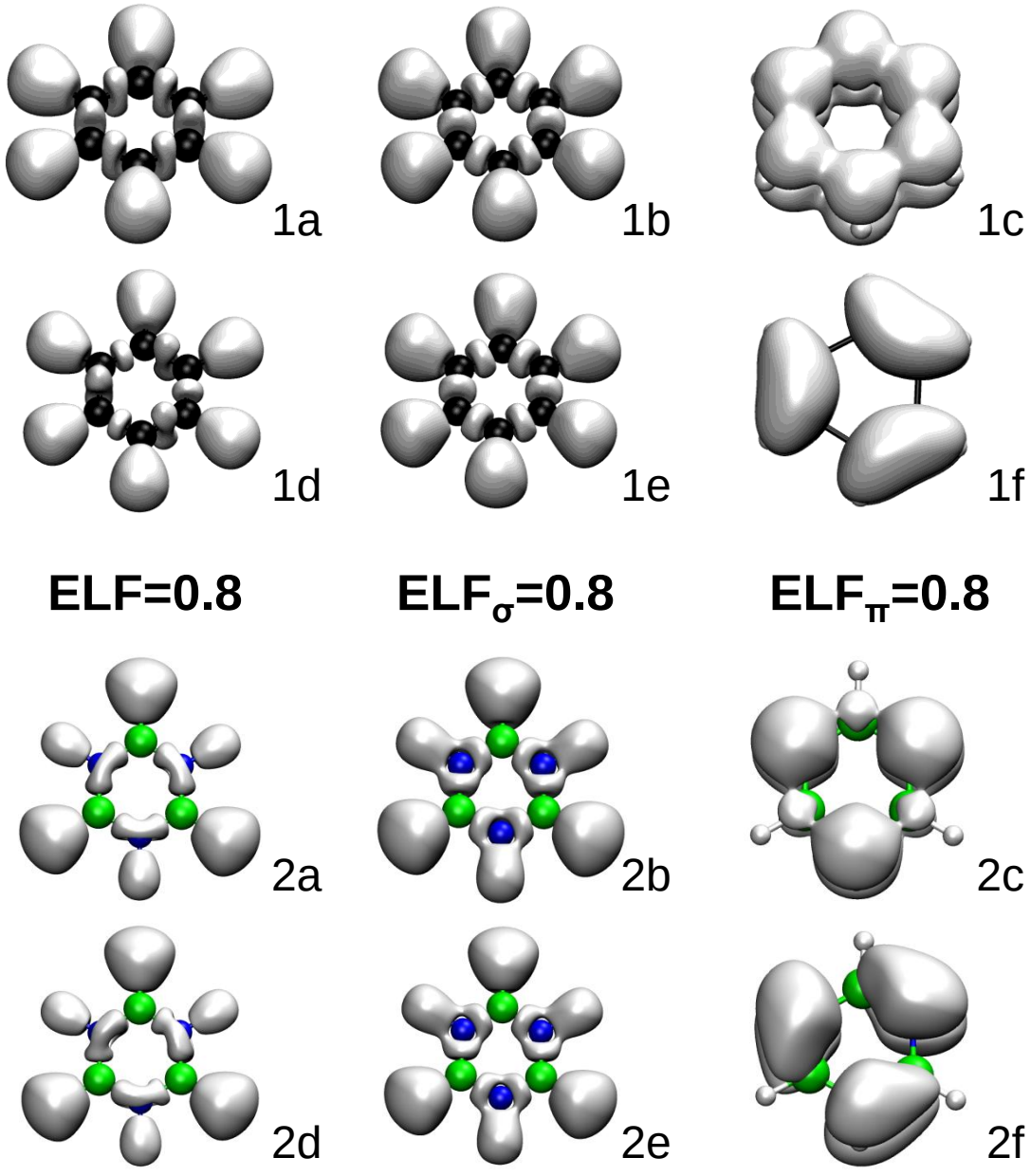


Figure S1 ELF isosurfaces (ELF=0.8) for benzene (1) and borazine (2). Boron and nitrogen atoms are in green and blue, respectively. From left to right: total, σ and π electrons. Upper row: Canonical, lower row: BLW.

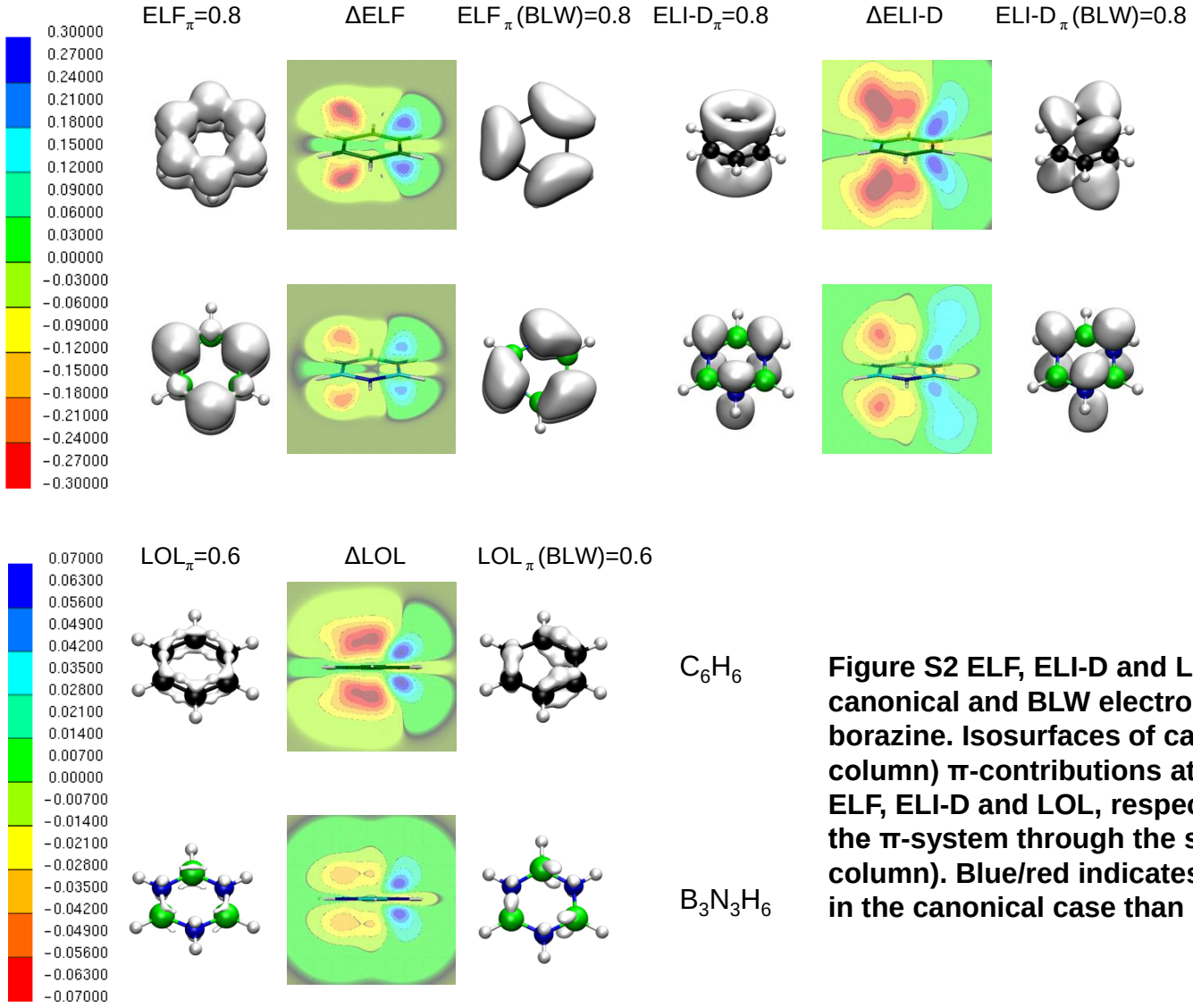


Figure S2 ELF, ELI-D and LOL differences between canonical and BLW electronic structure for benzene and borazine. Isosurfaces of canonical (1st column) and BLW (3rd column) π-contributions at a value of 0.8, 0.8 and 0.6 for ELF, ELI-D and LOL, respectively. Profiles perpendicular to the π-system through the single and double bond (2nd column). Blue/red indicates regions of higher/lower values in the canonical case than in BLW.

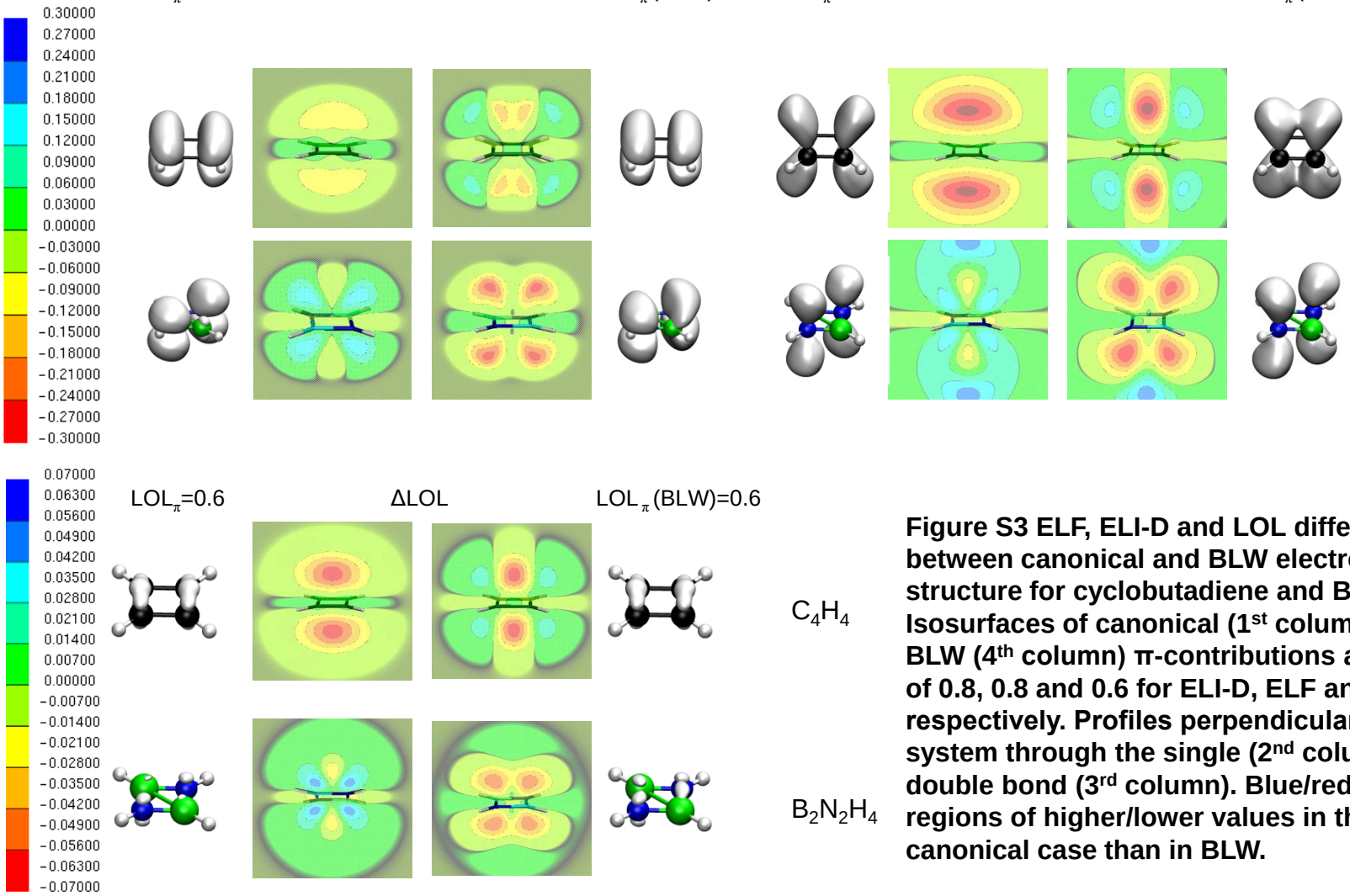


Figure S3 ELF, ELI-D and LOL differences between canonical and BLW electronic structure for cyclobutadiene and $B_2N_2H_4$. Isosurfaces of canonical (1st column) and BLW (4th column) π-contributions at a value of 0.8, 0.8 and 0.6 for ELI-D, ELF and LOL, respectively. Profiles perpendicular to the π-system through the single (2nd column) and double bond (3rd column). Blue/red indicates regions of higher/lower values in the canonical case than in BLW.

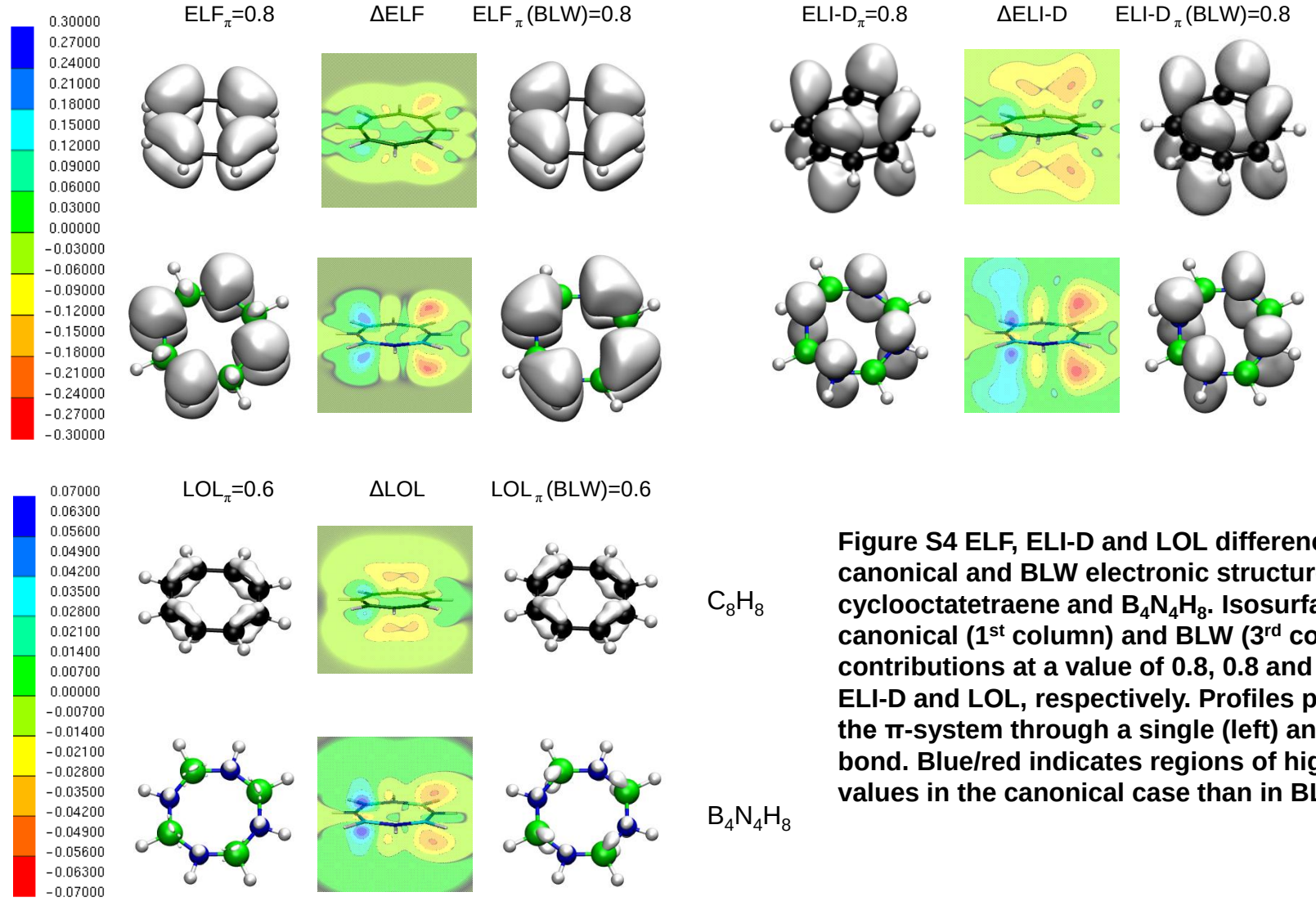
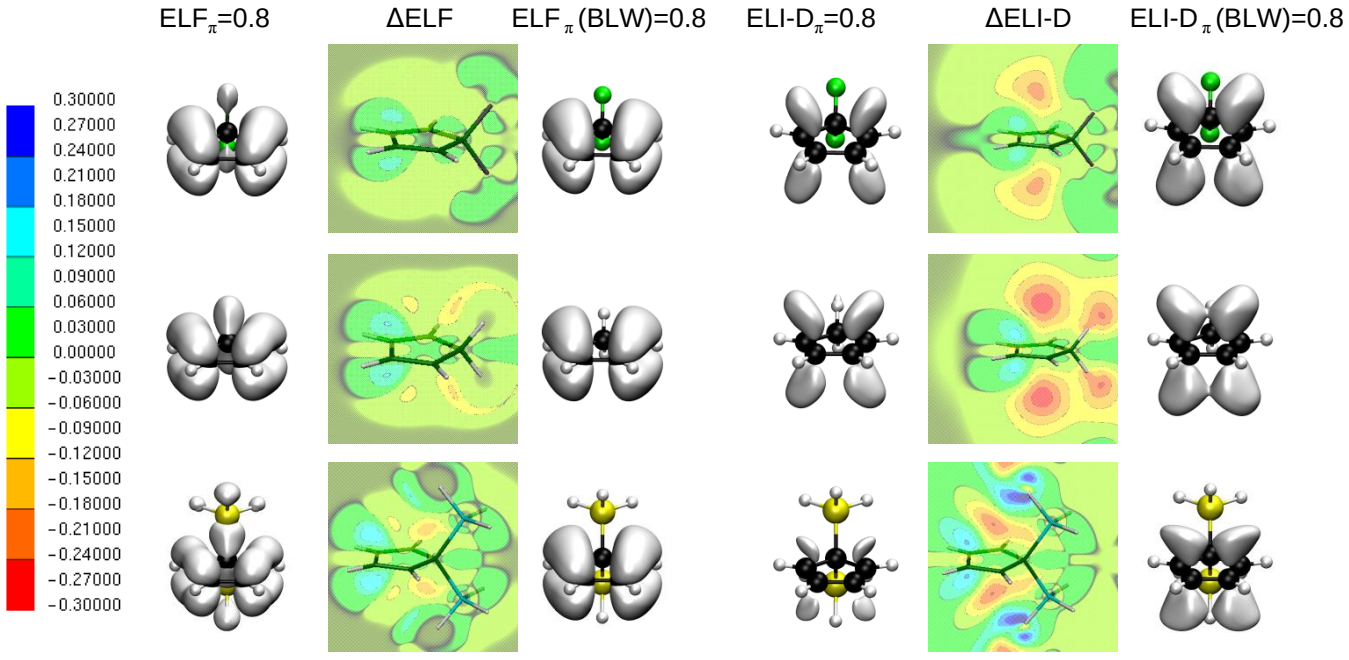


Figure S4 ELF, ELI-D and LOL differences between canonical and BLW electronic structure for cyclooctatetraene and $B_4N_4H_8$. Isosurfaces of canonical (1st column) and BLW (3rd column) π-contributions at a value of 0.8, 0.8 and 0.6 for ELF, ELI-D and LOL, respectively. Profiles perpendicular to the π-system through a single (left) and double (right) bond. Blue/red indicates regions of higher/lower values in the canonical case than in BLW.



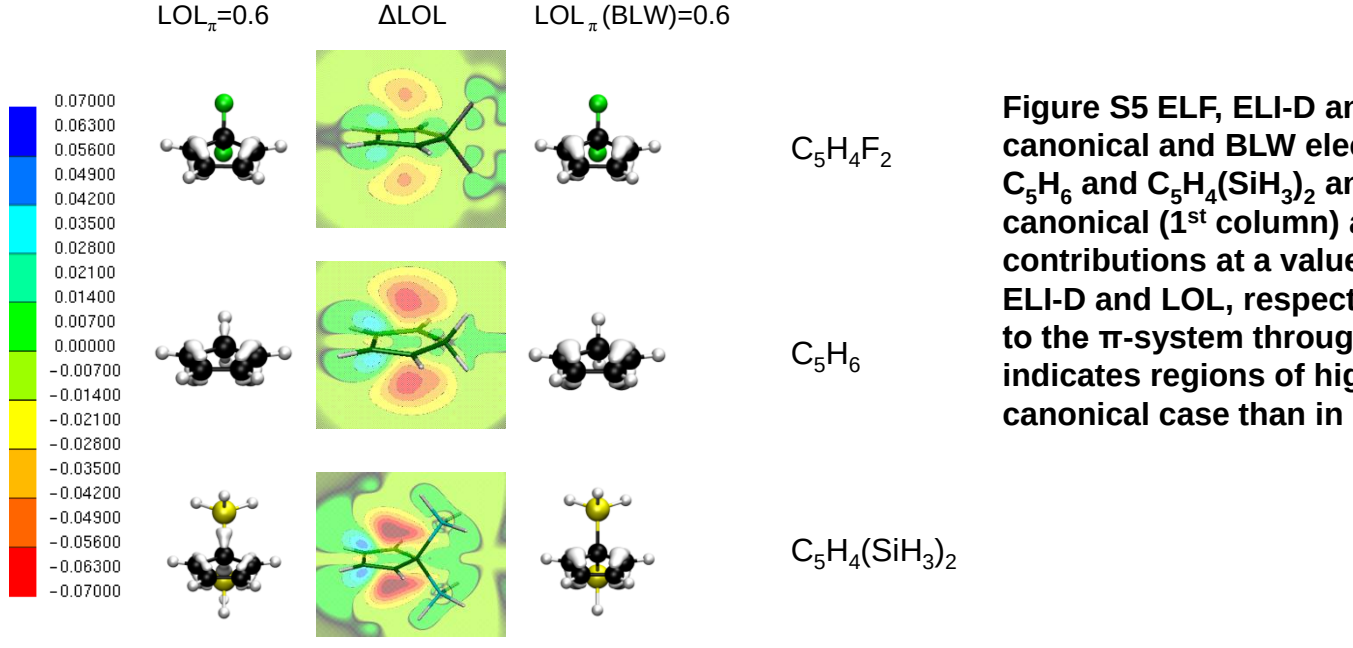


Figure S5 ELF, ELI-D and LOL differences between canonical and BLW electronic structure for $C_5H_4F_2$, C_5H_6 and $C_5H_4(SiH_3)_2$ and borazine. Isosurfaces of canonical (1st column) and BLW (3rd column) π-contributions at a value of 0.8, 0.8 and 0.6 for ELF, ELI-D and LOL, respectively. Profiles perpendicular to the π-system through the single bond. Blue/red indicates regions of higher/lower values in the canonical case than in BLW.

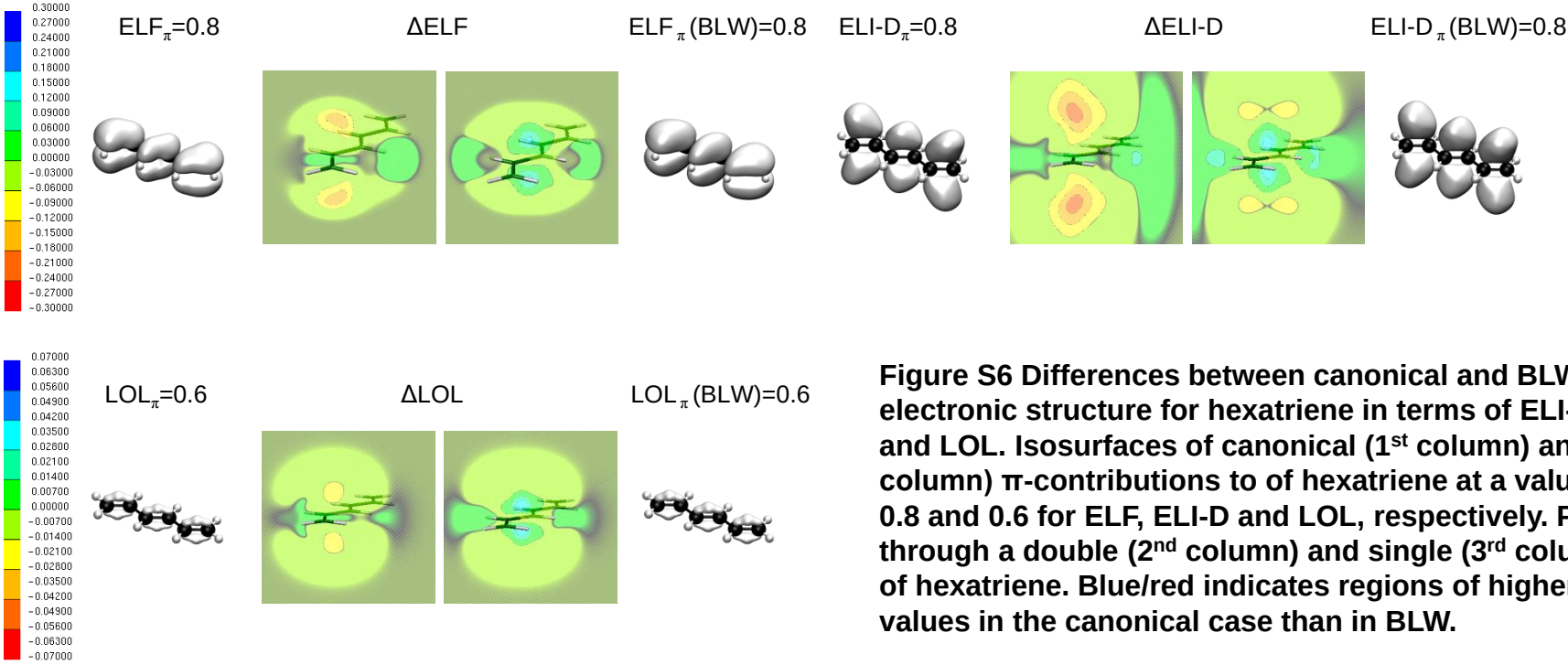


Figure S6 Differences between canonical and BLW electronic structure for hexatriene in terms of ELI-D, ELF and LOL. Isosurfaces of canonical (1st column) and BLW (4th column) π-contributions to of hexatriene at a value of 0.8, 0.8 and 0.6 for ELF, ELI-D and LOL, respectively. Profiles through a double (2nd column) and single (3rd column) bond of hexatriene. Blue/red indicates regions of higher/lower values in the canonical case than in BLW.

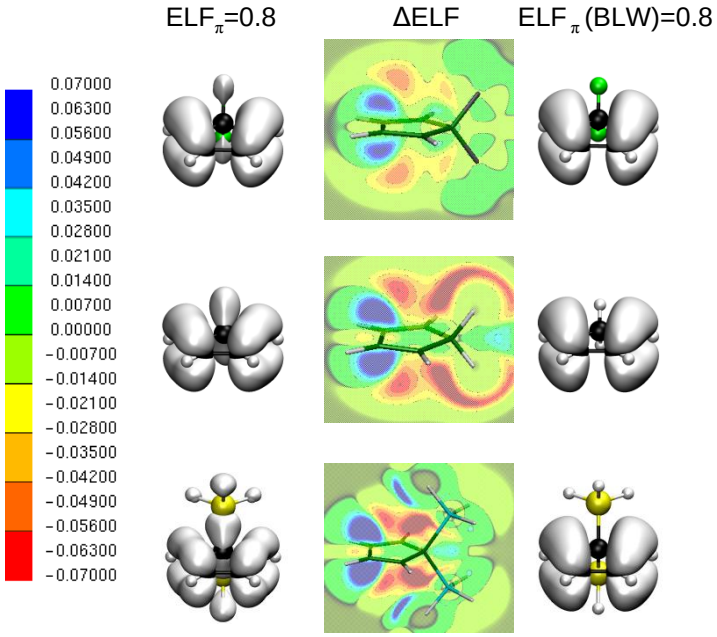


Figure S7 ELF differences between canonical and BLW electronic structure for $C_5H_4F_2$, C_5H_6 and $C_5H_4(SiH_3)_2$ and borazine. Isosurfaces of canonical (1st column) and BLW (3rd column) π-contributions at a value of 0.8 for ELF. Profiles perpendicular to the π-system through the single bond. Blue/red indicates regions of higher/lower values in the canonical case than in BLW.