

Supplementary information: The effect of complex optimal orbitals on atomization energies with the Perdew–Zunger self-interaction correction to density functional theory

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The scatter plots for the atomization energy errors for the 10 functionals studied in the present work are shown in Figures 1 – 36. In each figure, the division of the molecules into classes (A), (B), (C), and (D) has been illustrated with a vertical dashed black line. The plots also show vertical, solid blue lines illustrating the mean error  $\mu$  in each class, as well as two vertical dashed, blue lines illustrating  $\mu - \sigma$  and  $\mu + \sigma$  where  $\sigma$  is the root mean square deviation within the class. The x axes show the name of the molecule in the W4-11 database.

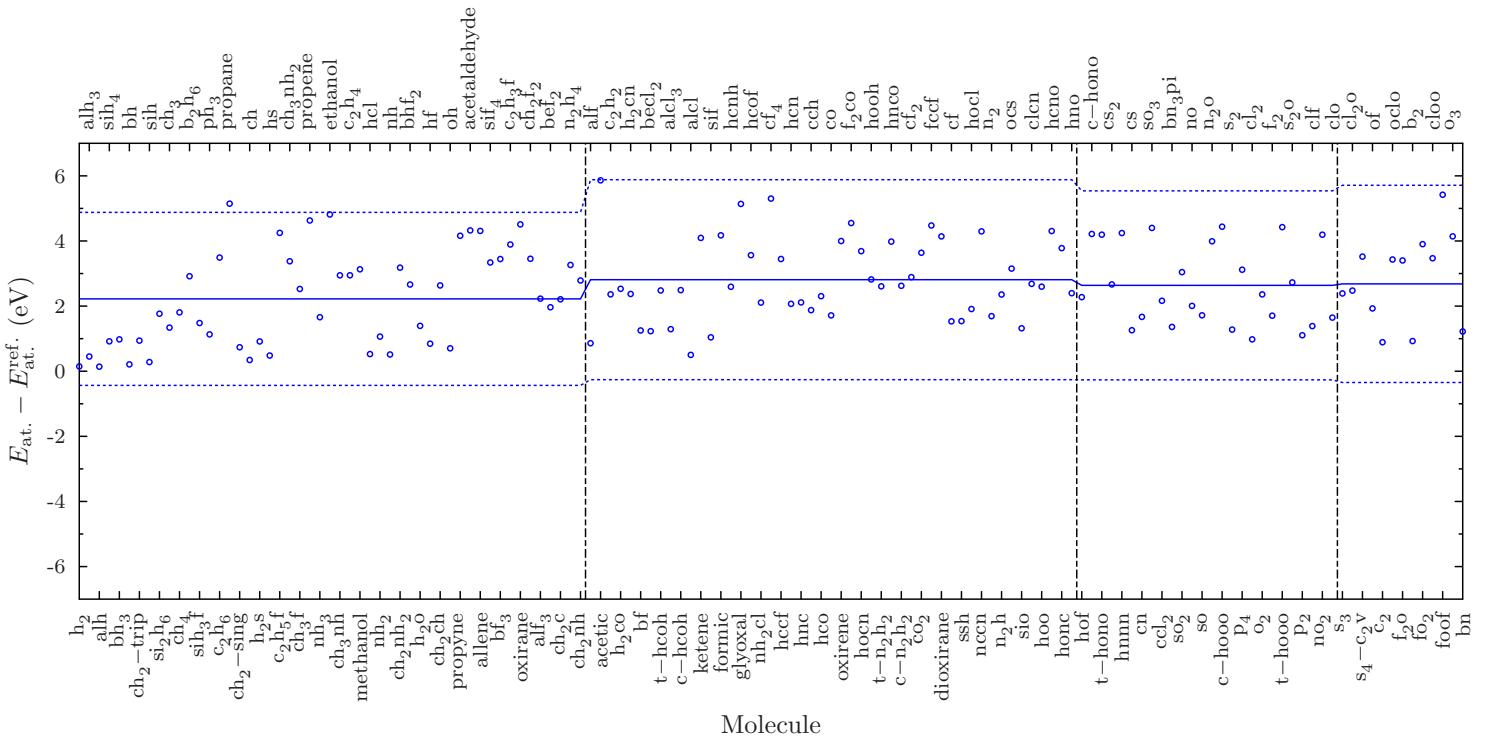


Figure 1: LDA KS-DFT results.

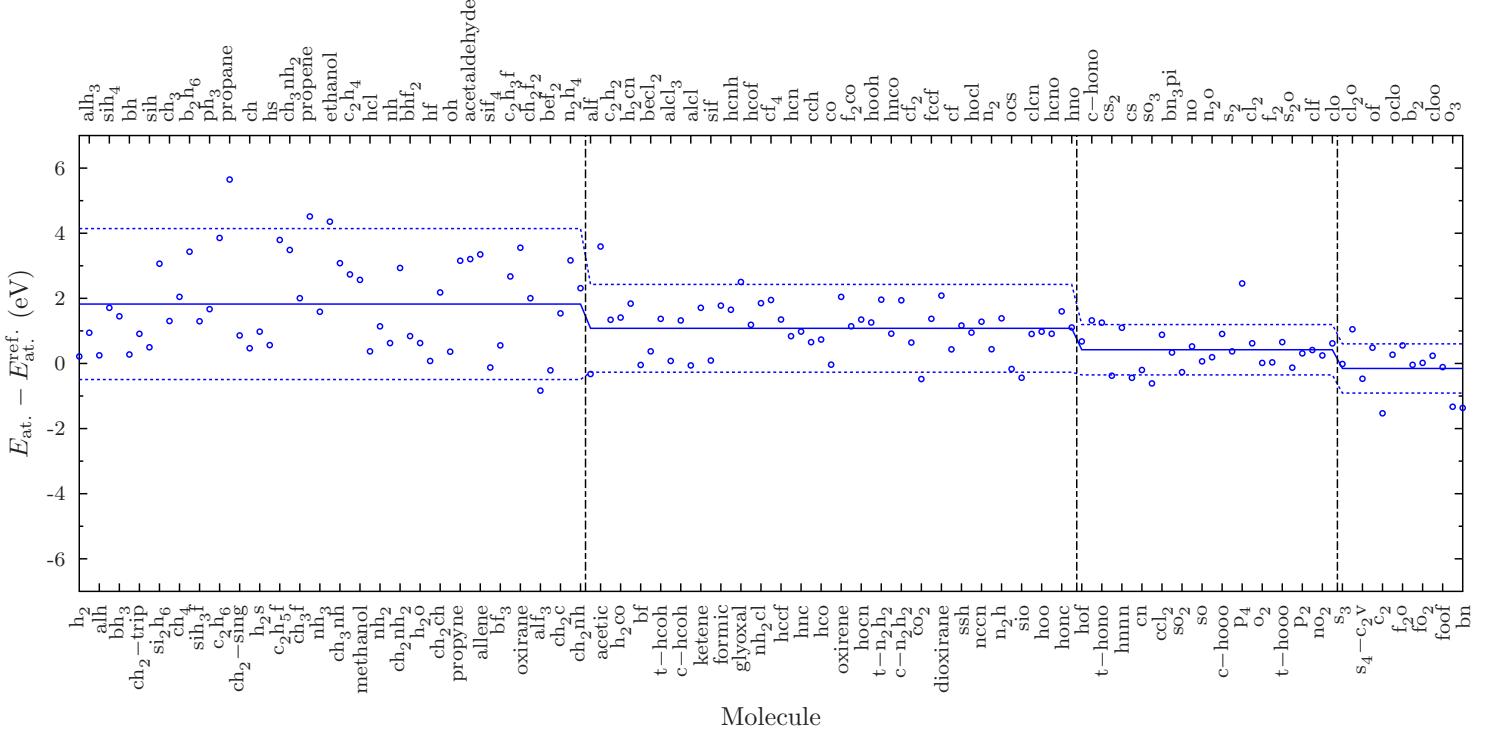


Figure 2: LDA PZ-RSIC results.

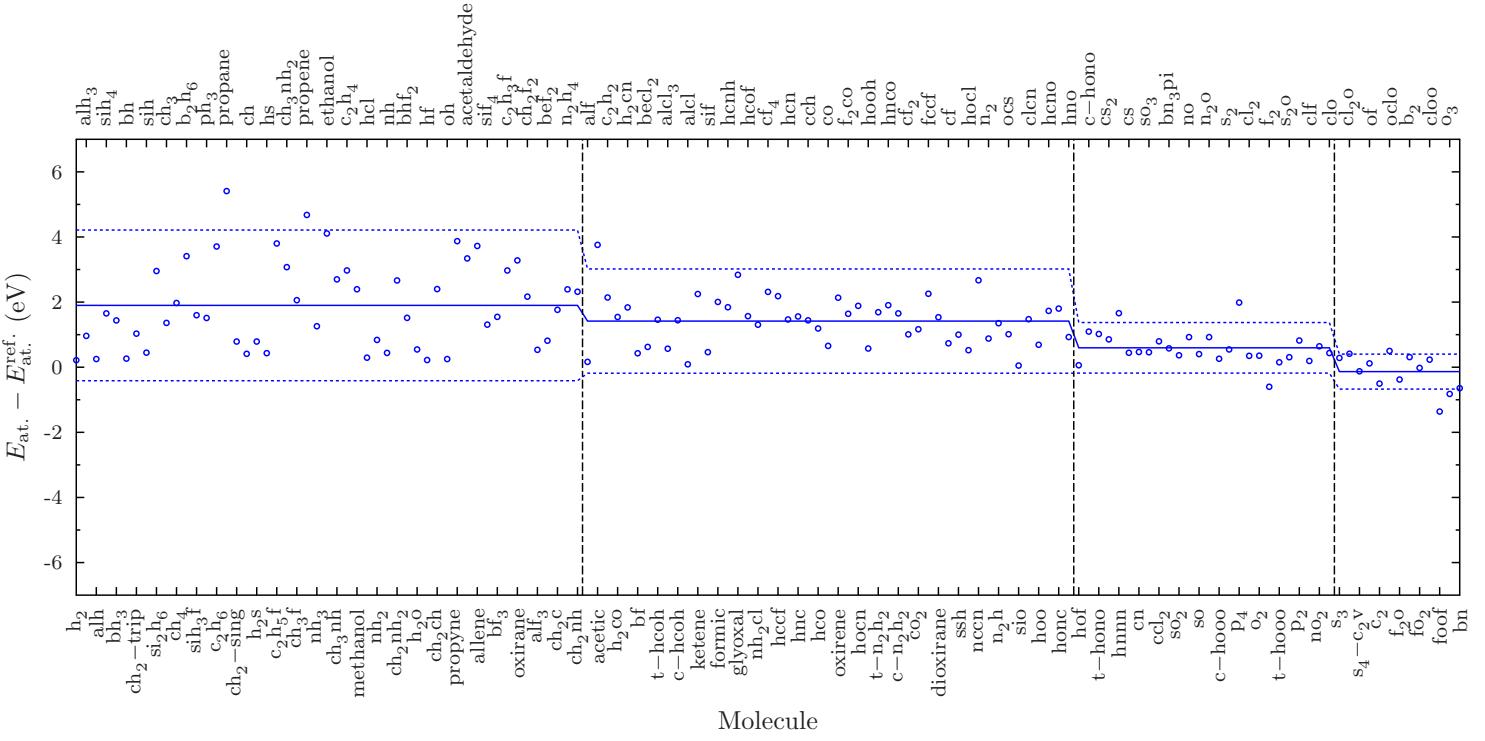


Figure 3: LDA PZ-SIC results.

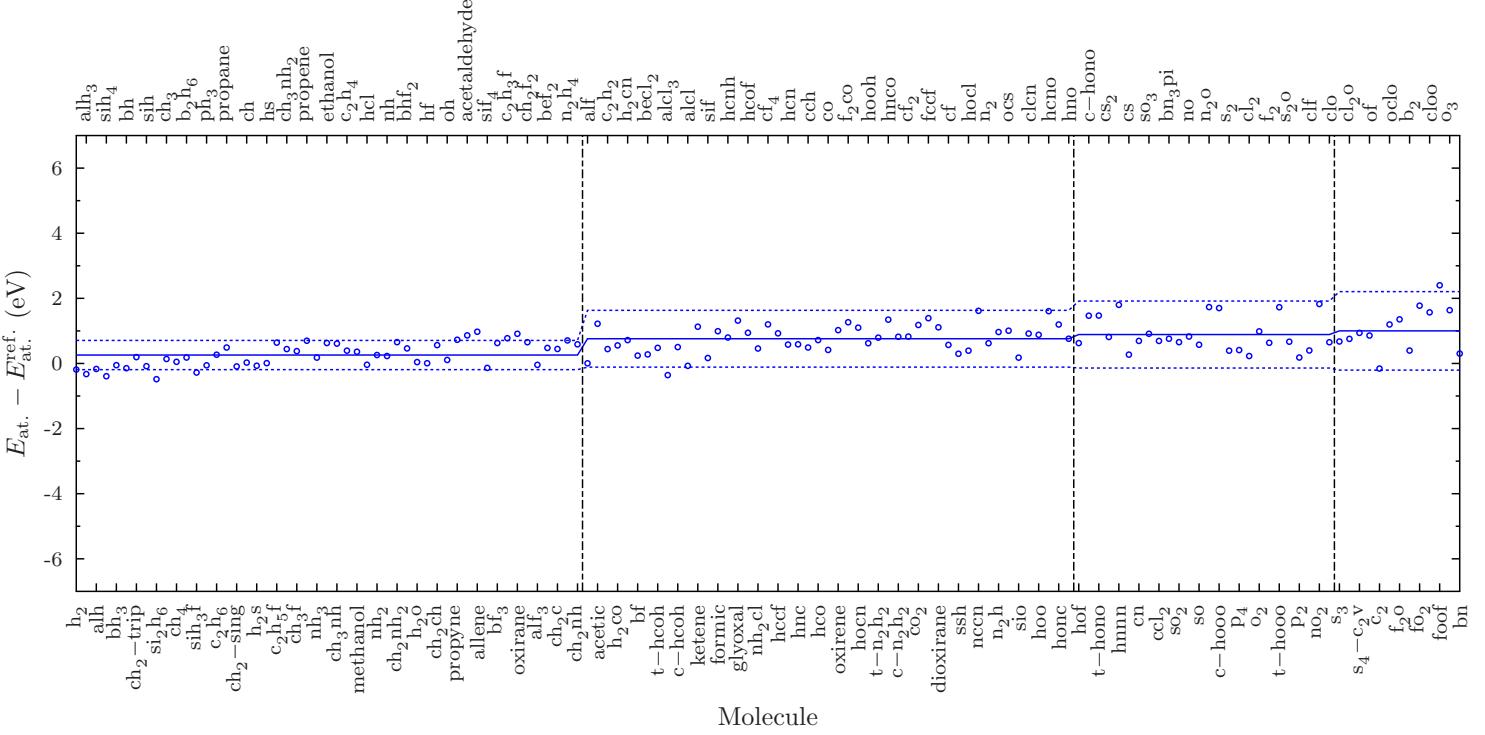


Figure 4: PW91 KS-DFT results.

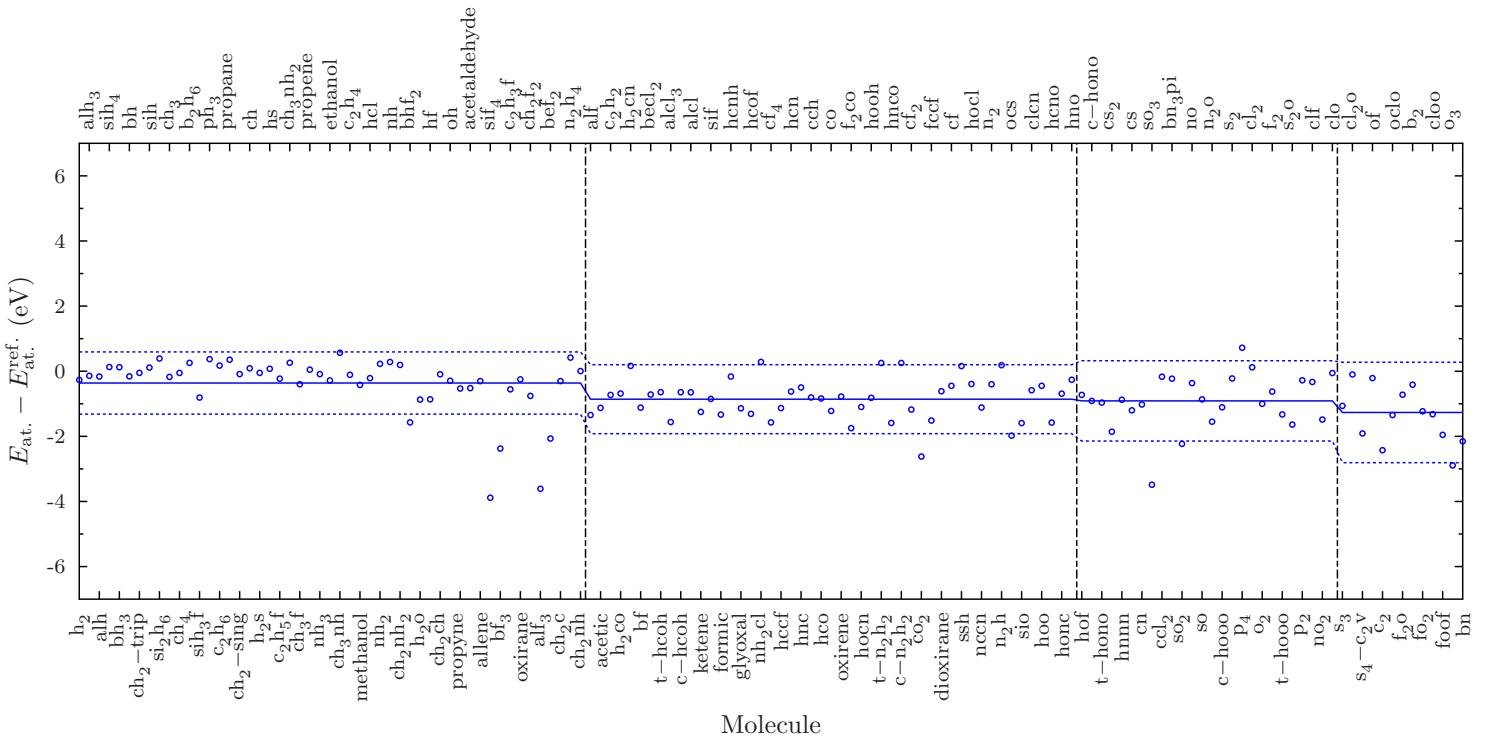


Figure 5: PW91 PZ-RSIC results.

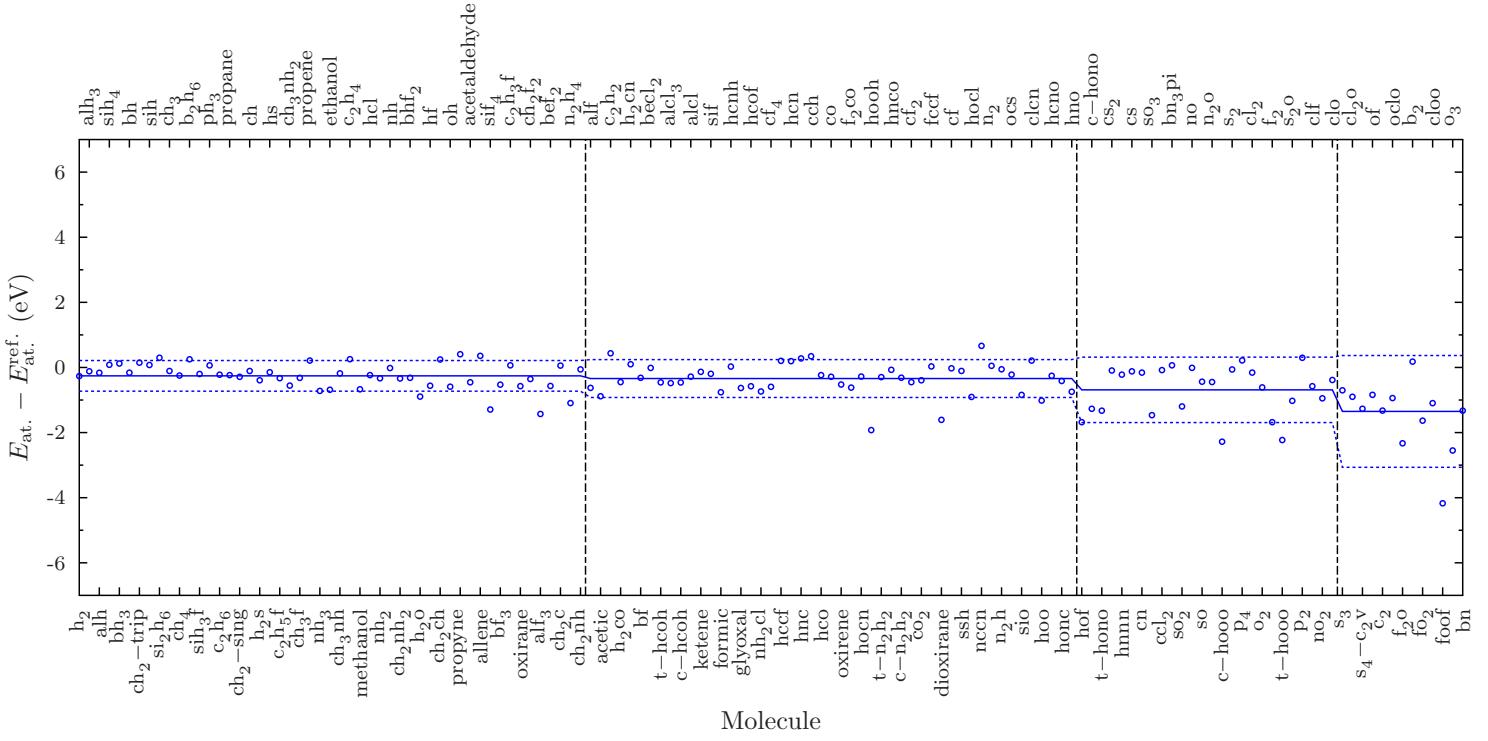


Figure 6: PW91 PZ-SIC results.

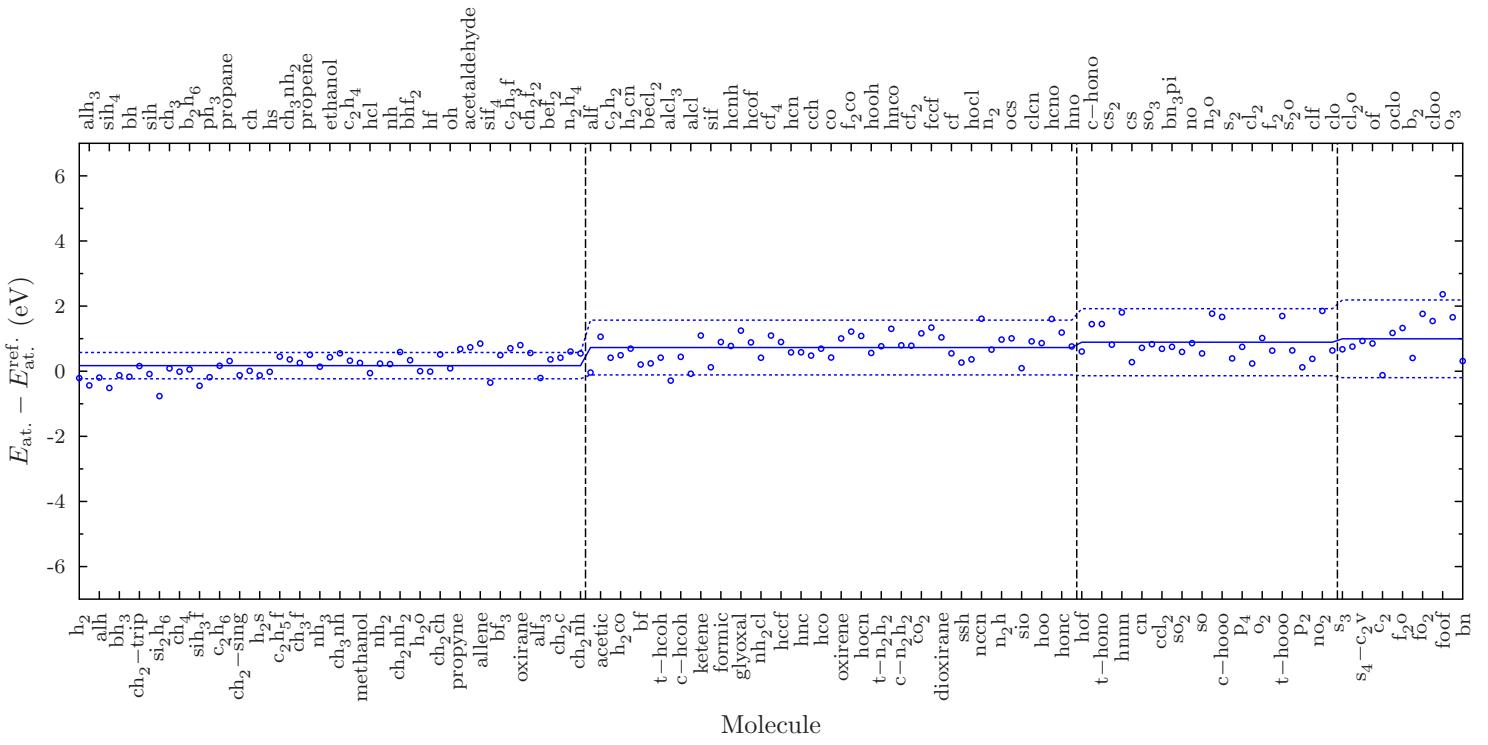


Figure 7: PBE KS-DFT results.

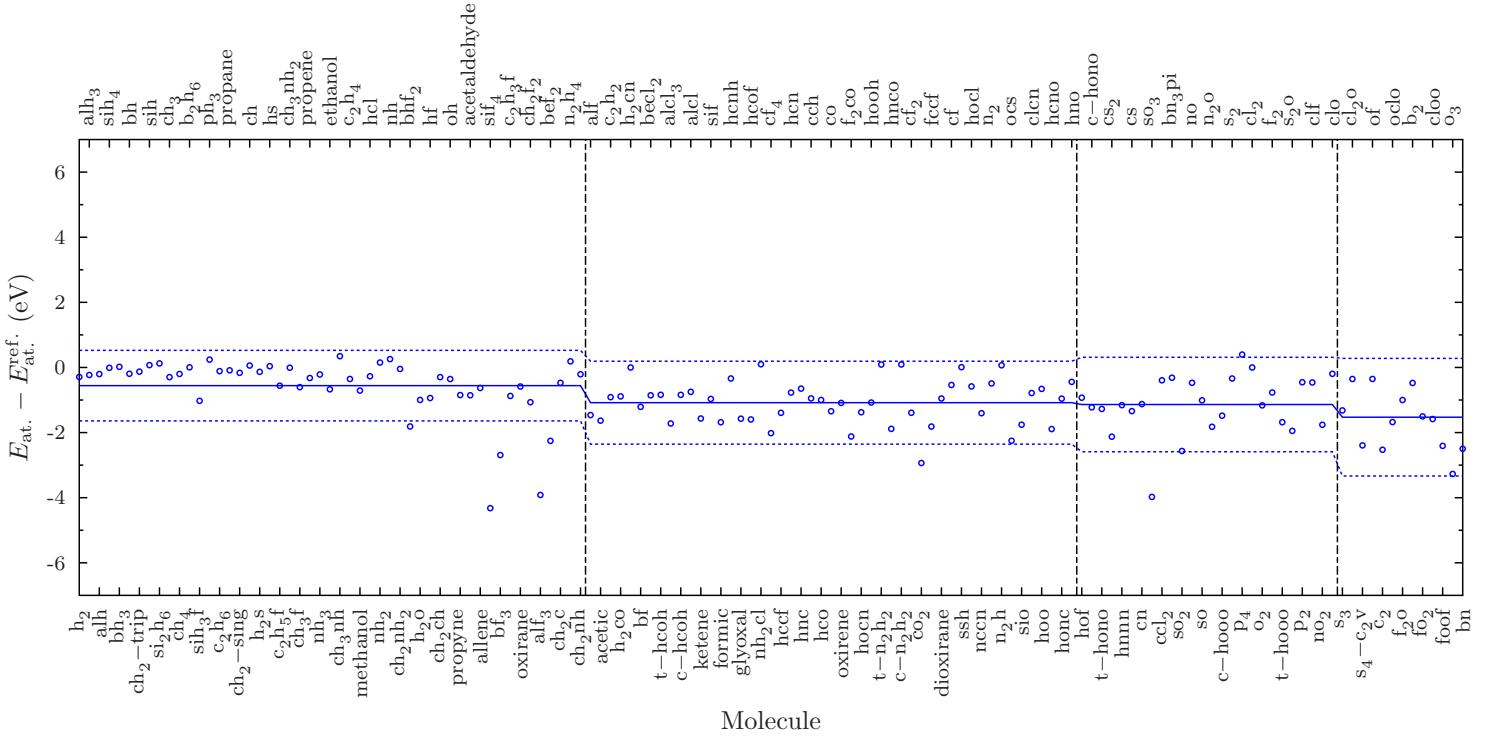


Figure 8: PBE PZ-RSIC results.

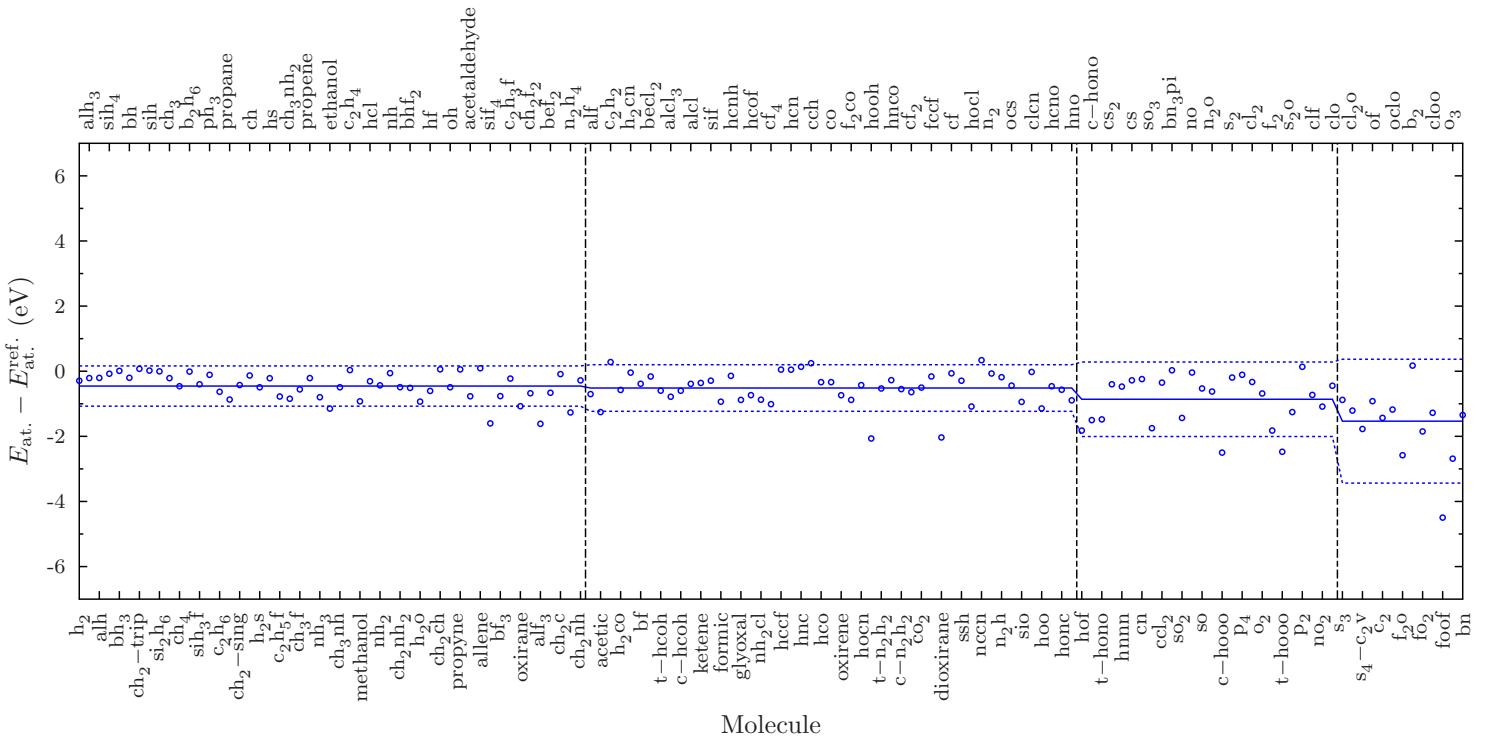


Figure 9: PBE PZ-SIC results.

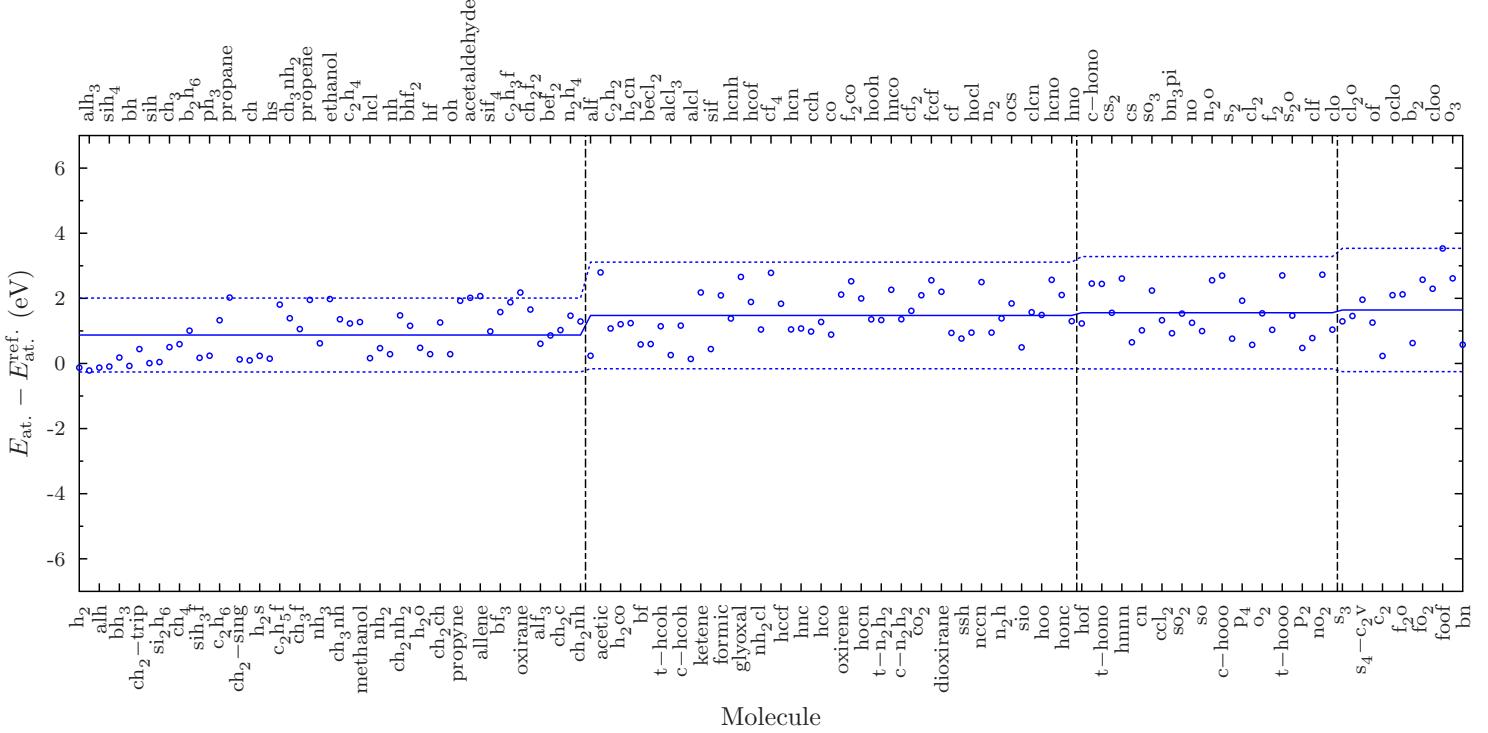


Figure 10: PBESol KS-DFT results.

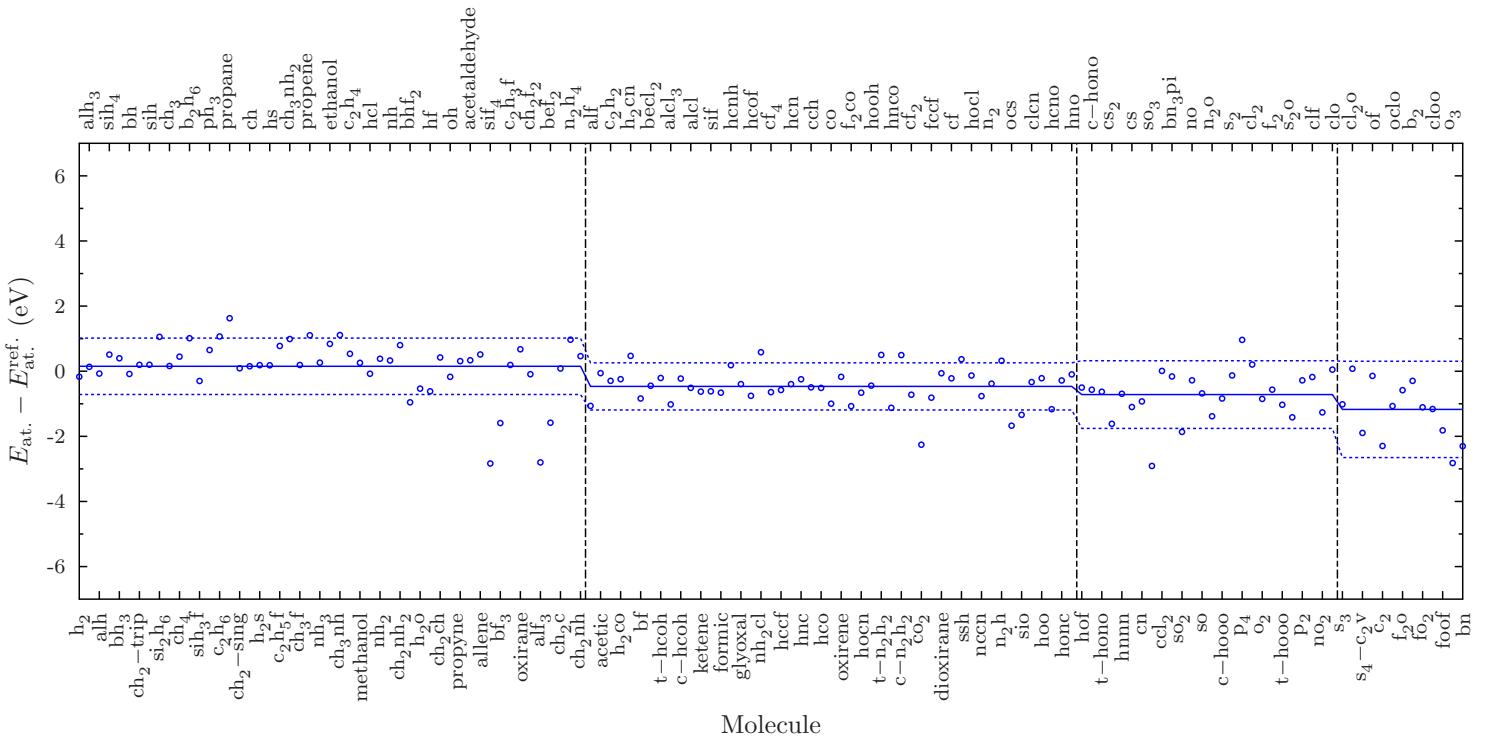


Figure 11: PBEsol PZ-RSIC results.

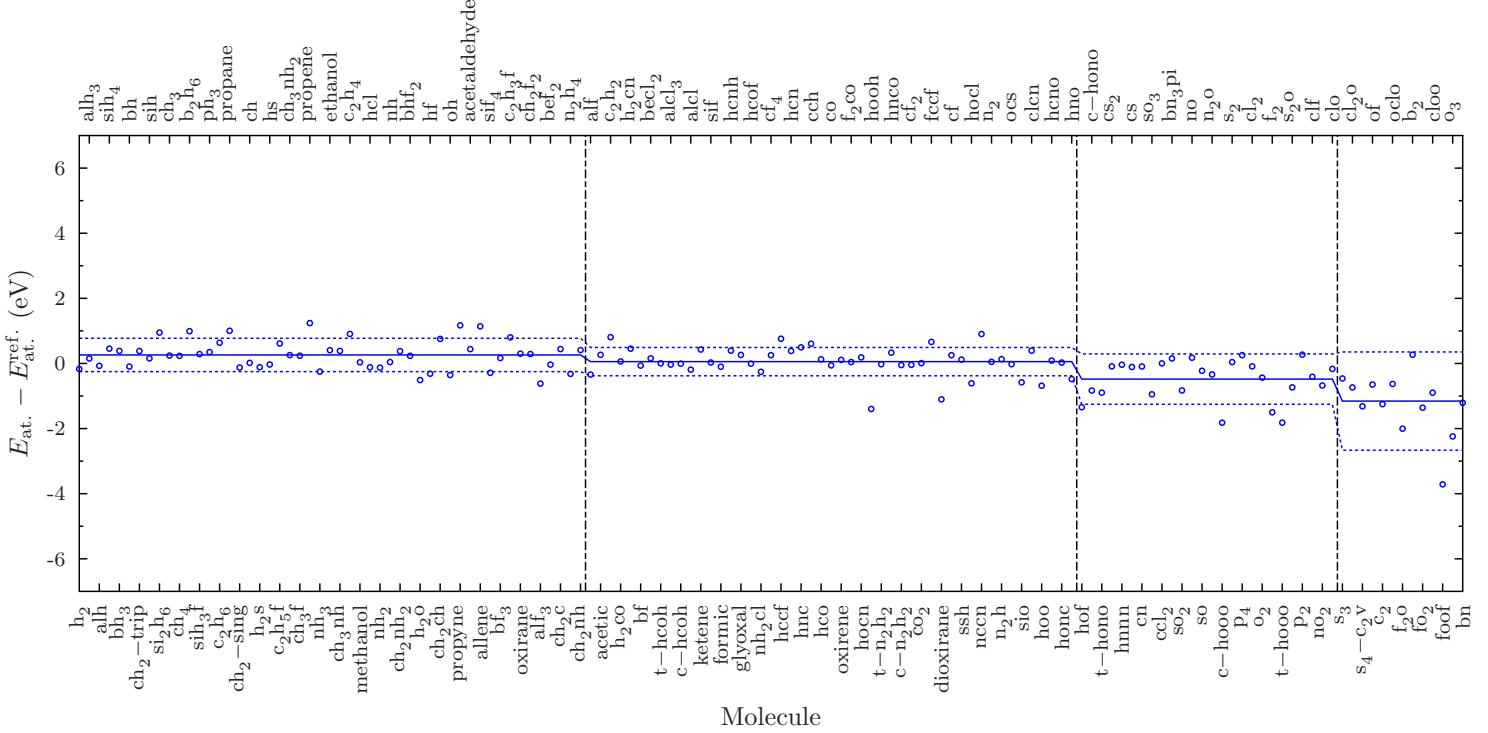


Figure 12: PBEsol PZ-SIC results.

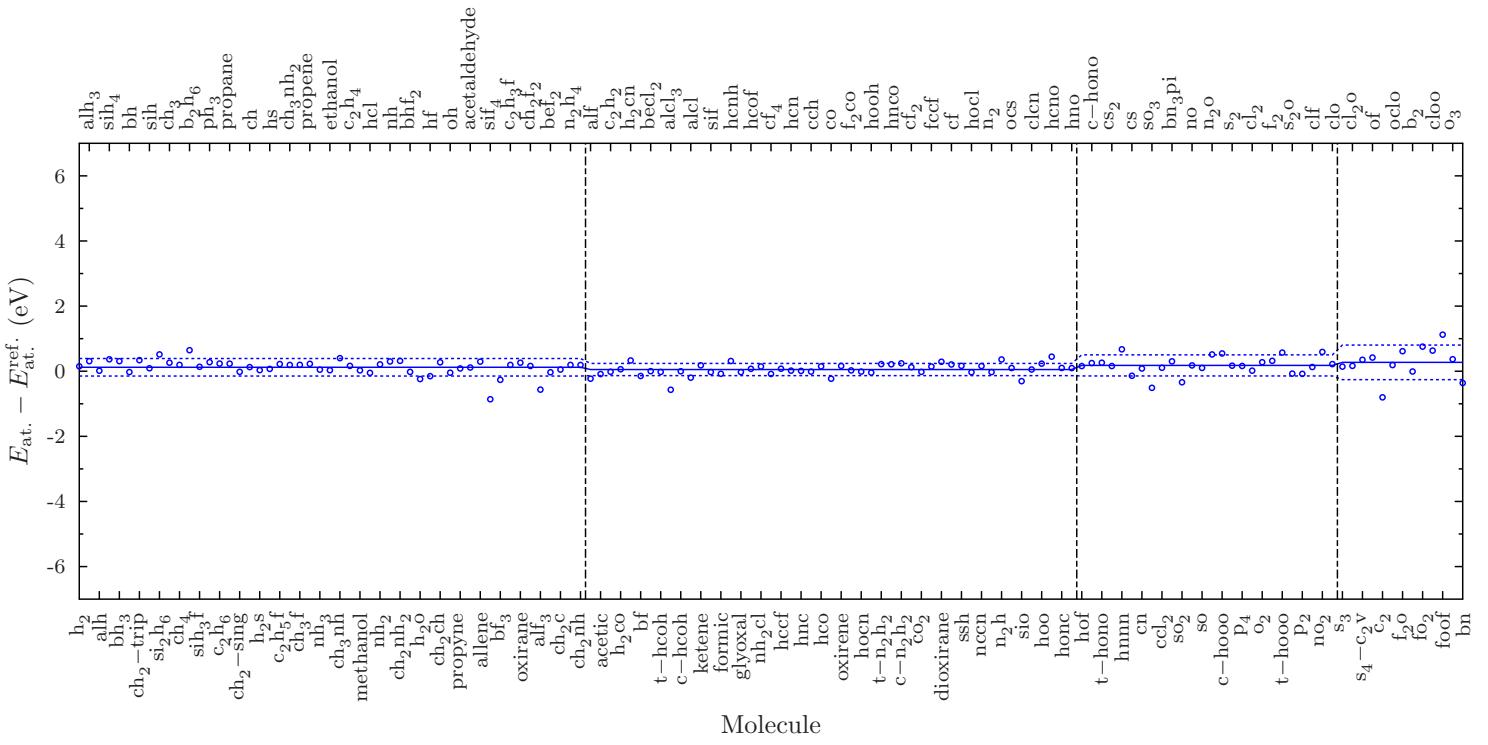


Figure 13: TPSS KS-DFT results.

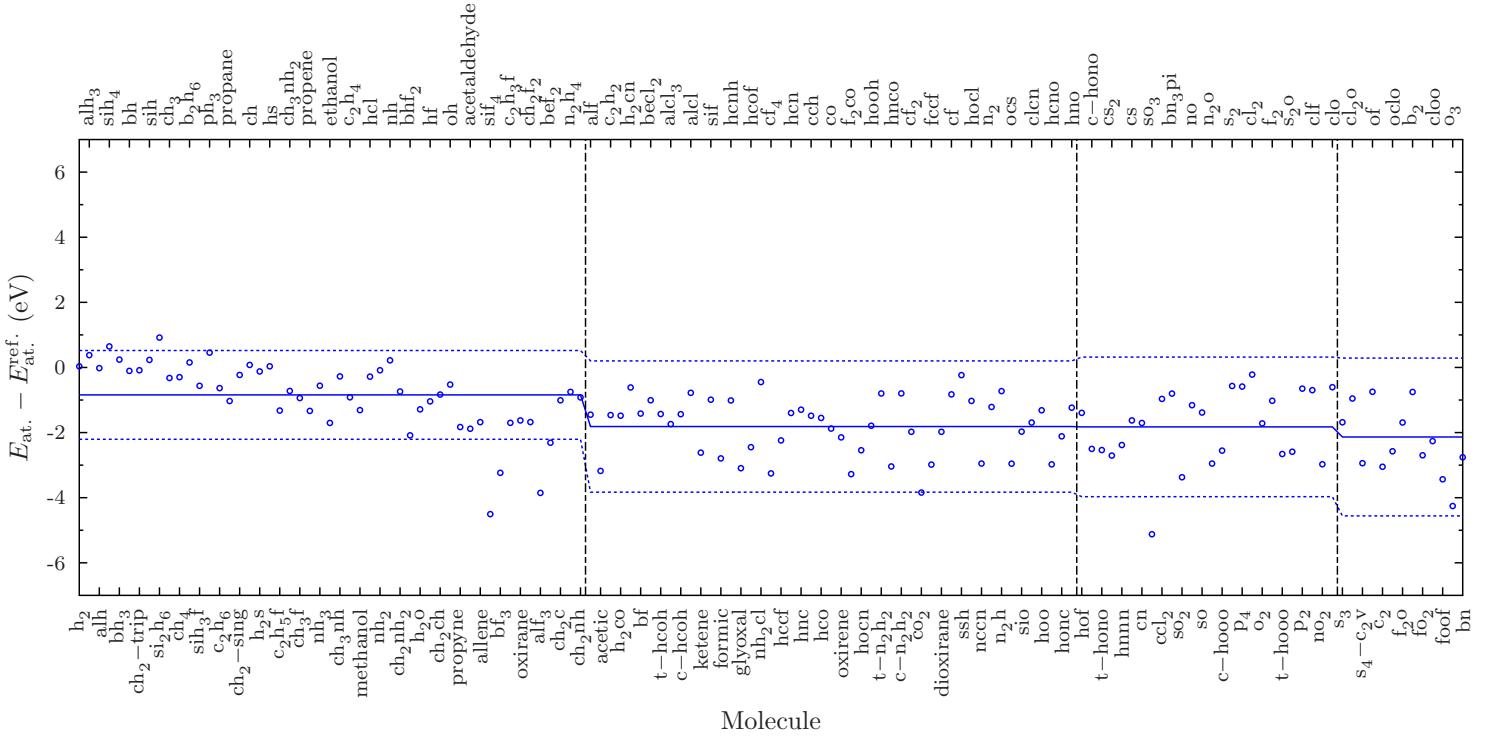


Figure 14: TPSS PZ-RSIC results.

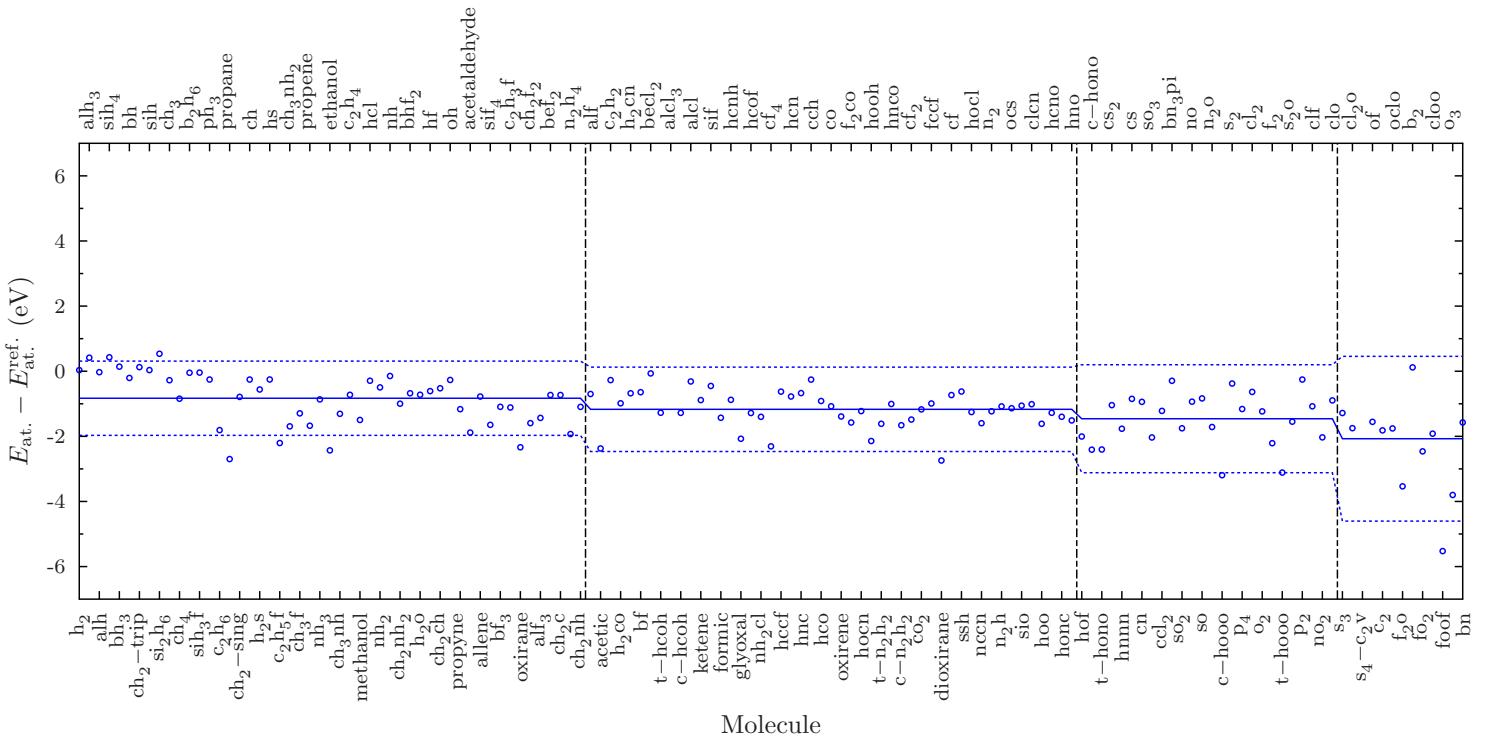


Figure 15: TPSS PZ-SIC results.

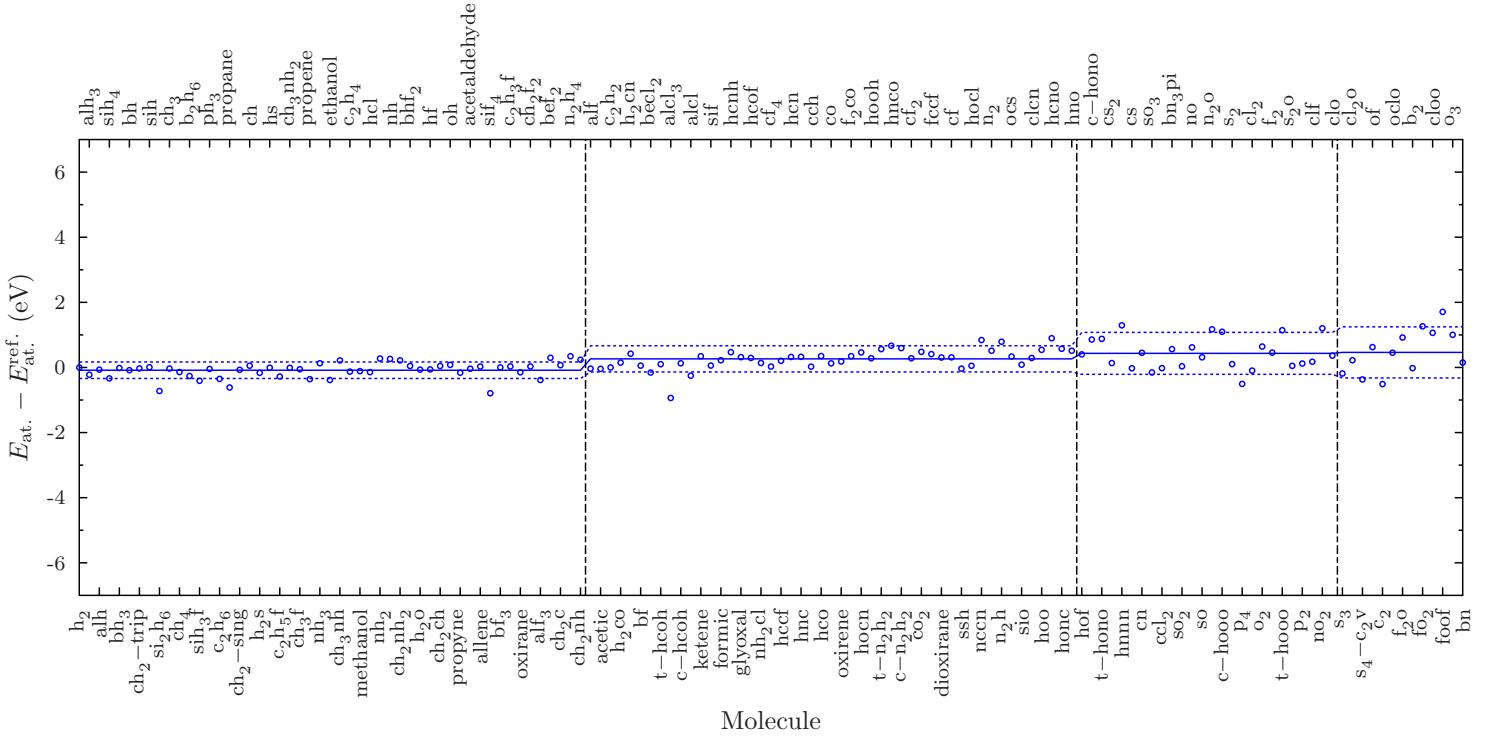


Figure 16: BLYP KS-DFT results.

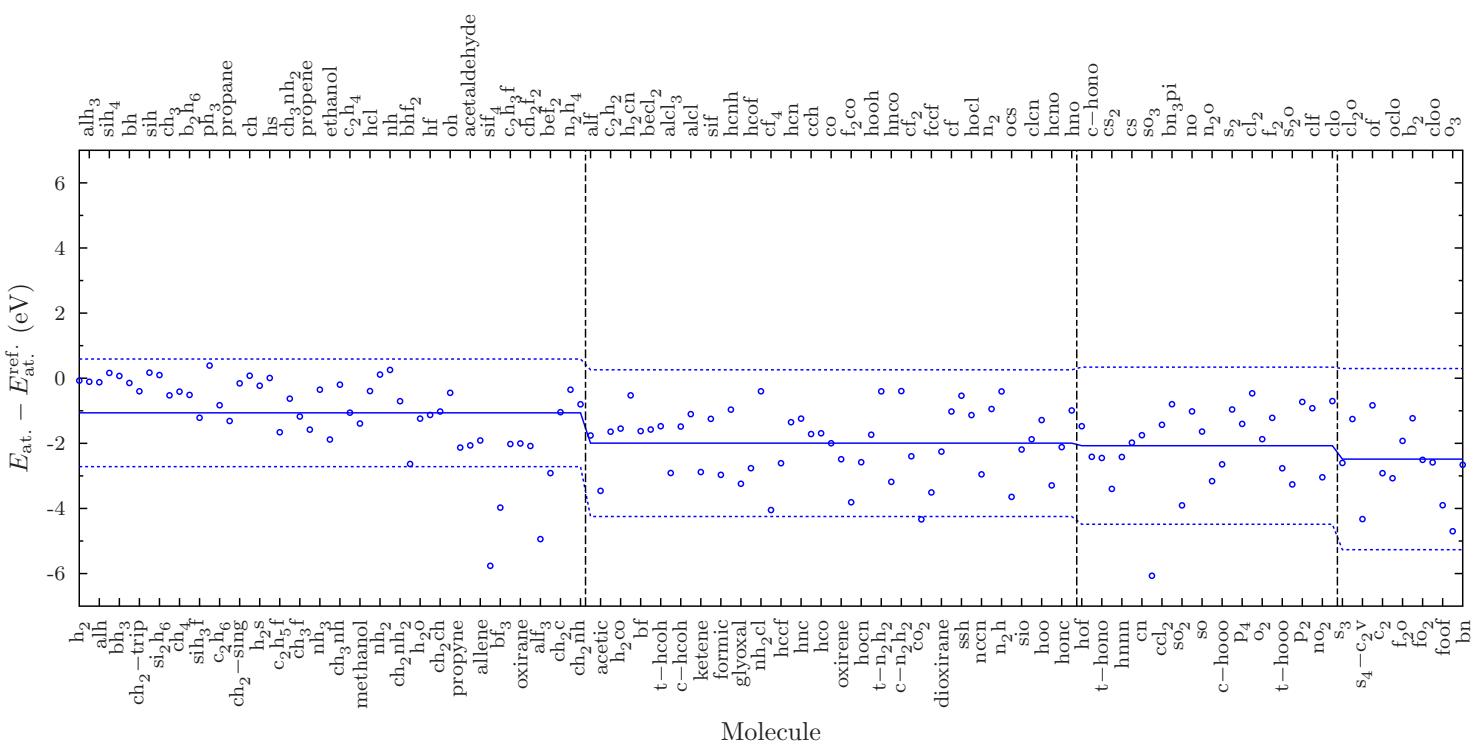


Figure 17: BLYP PZ-RSIC results.

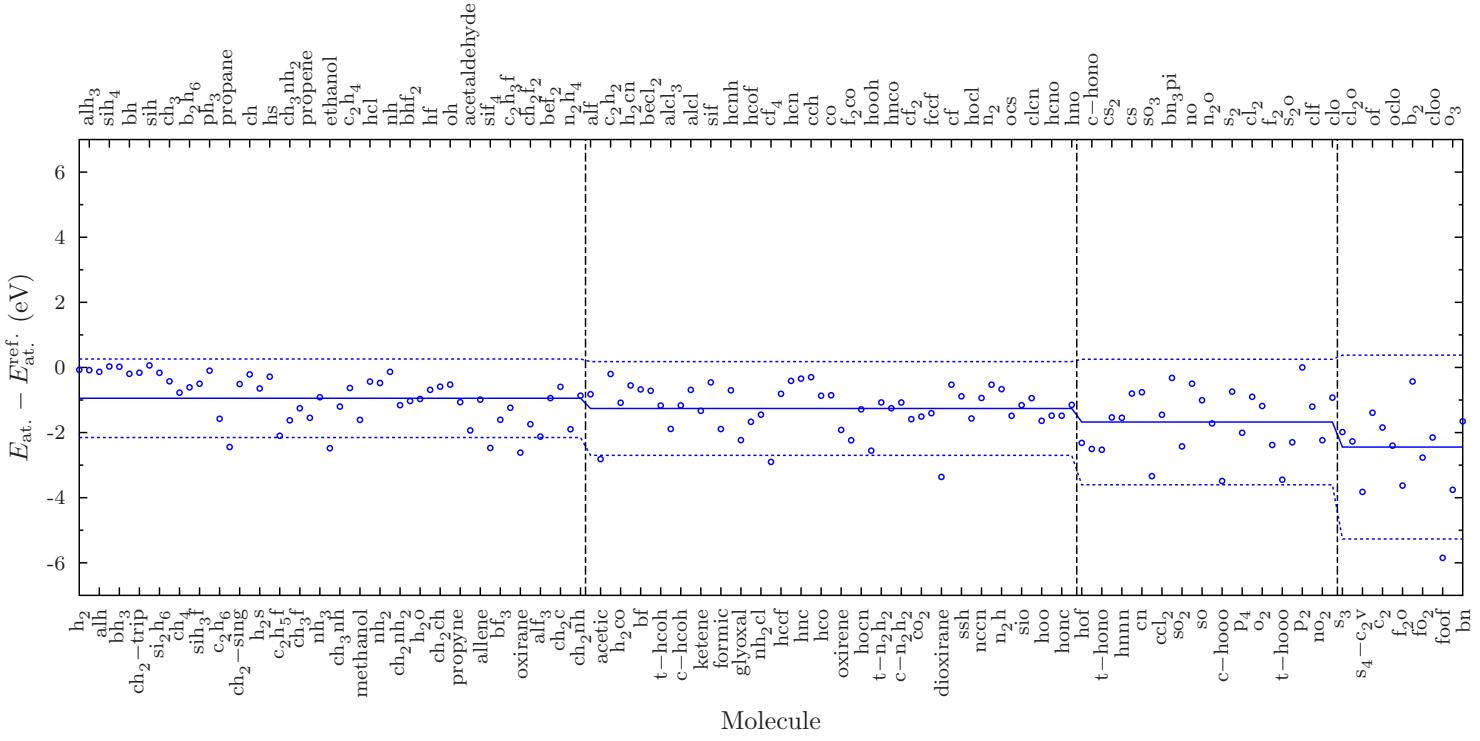


Figure 18: BLYP PZ-SIC results.

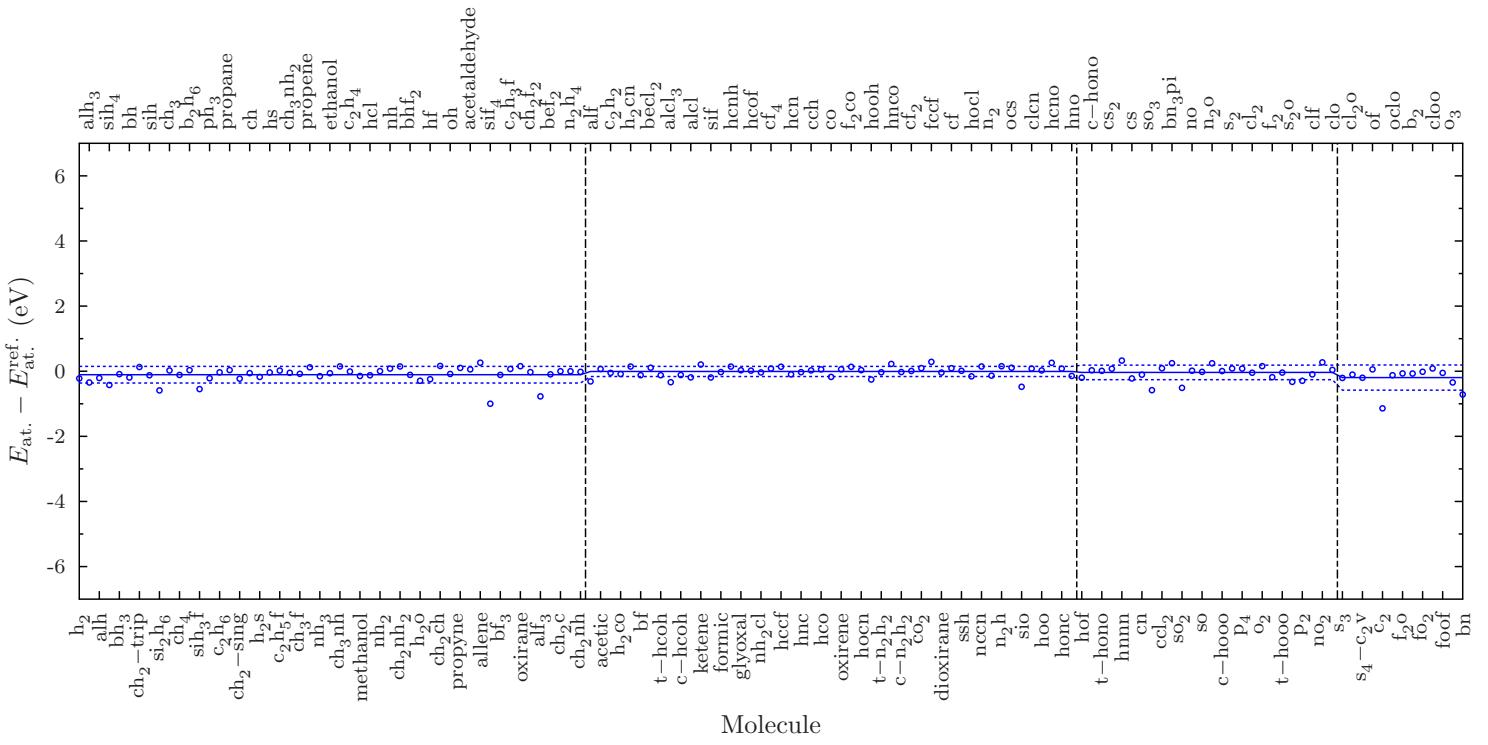


Figure 19: PBE0 KS-DFT results.

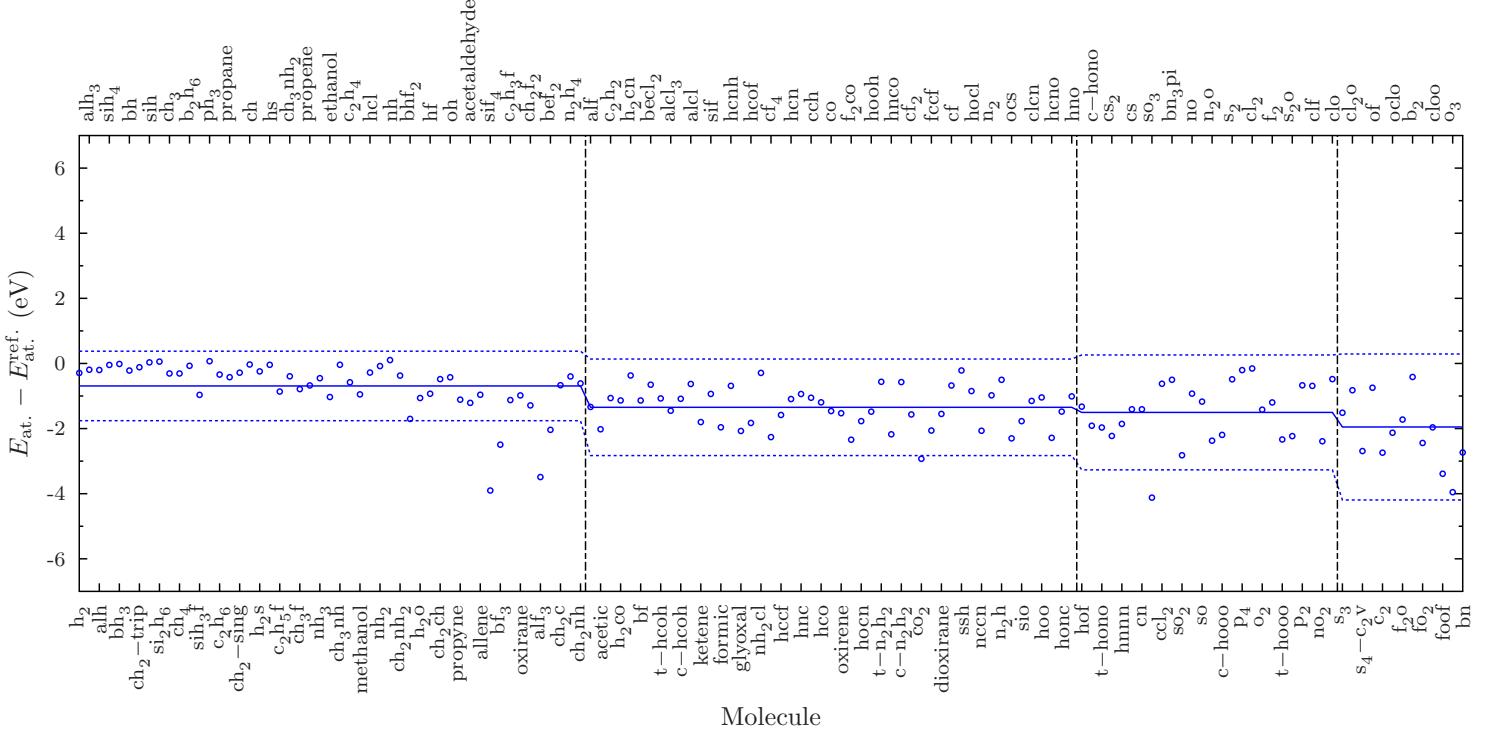


Figure 20: PBE0 PZ-RSIC results.

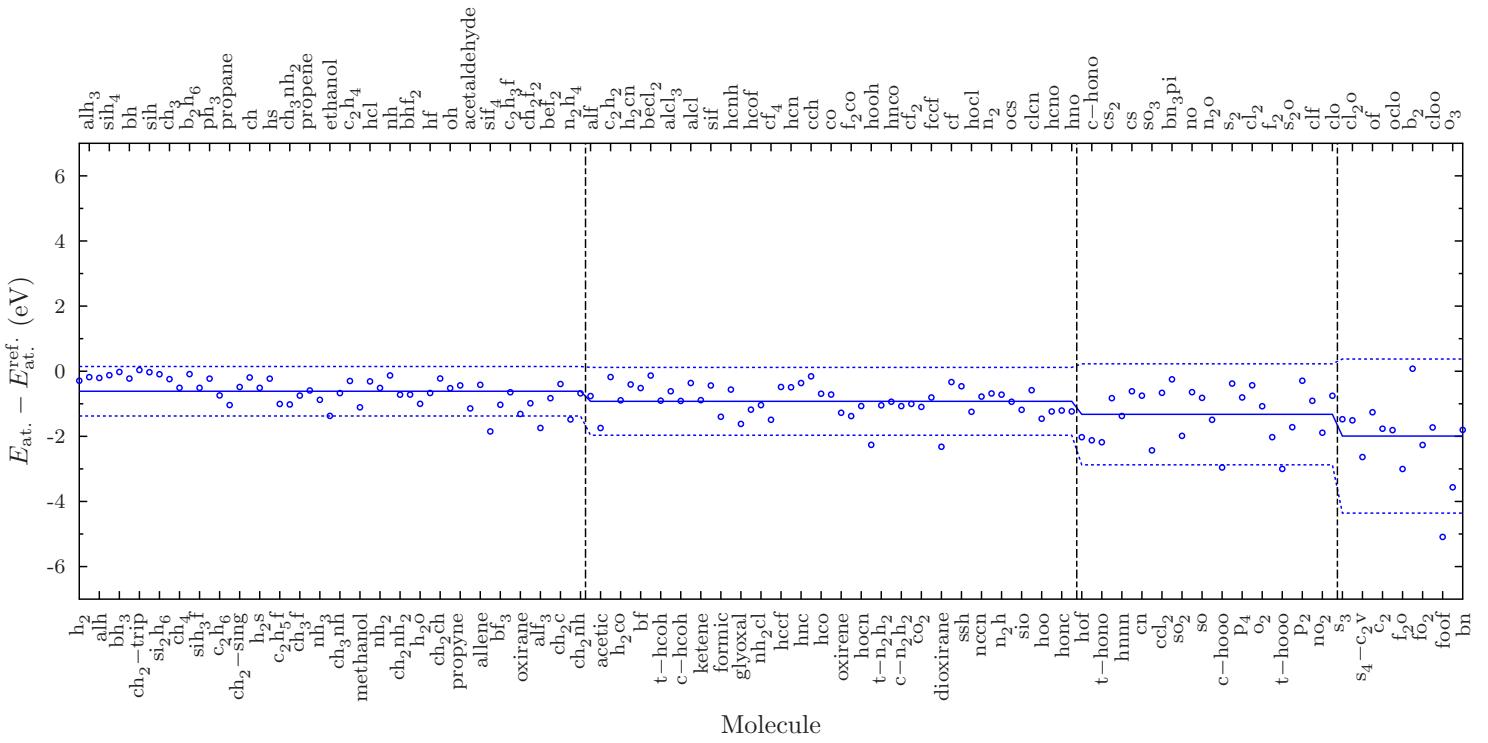


Figure 21: PBE0 PZ-SIC results.

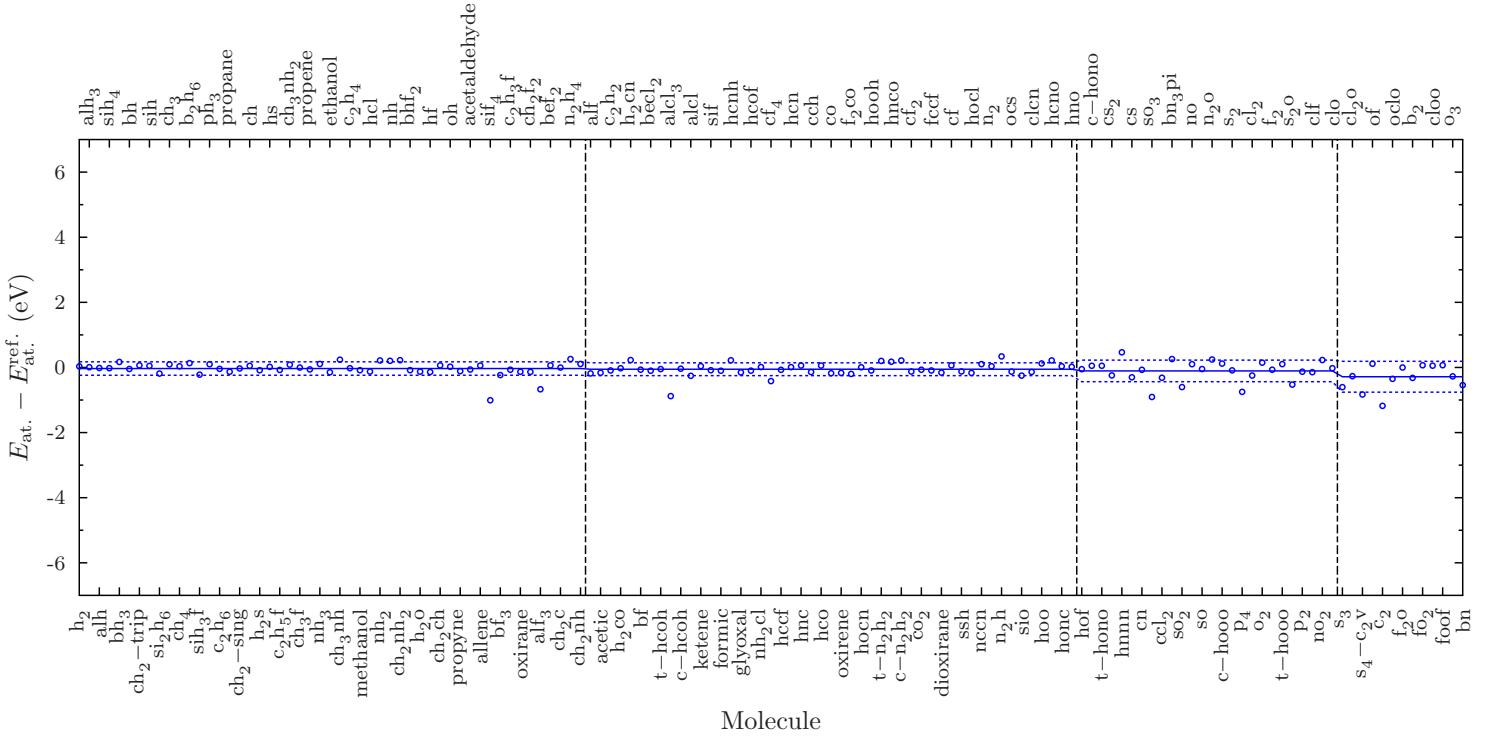


Figure 22: B3LYP KS-DFT results.

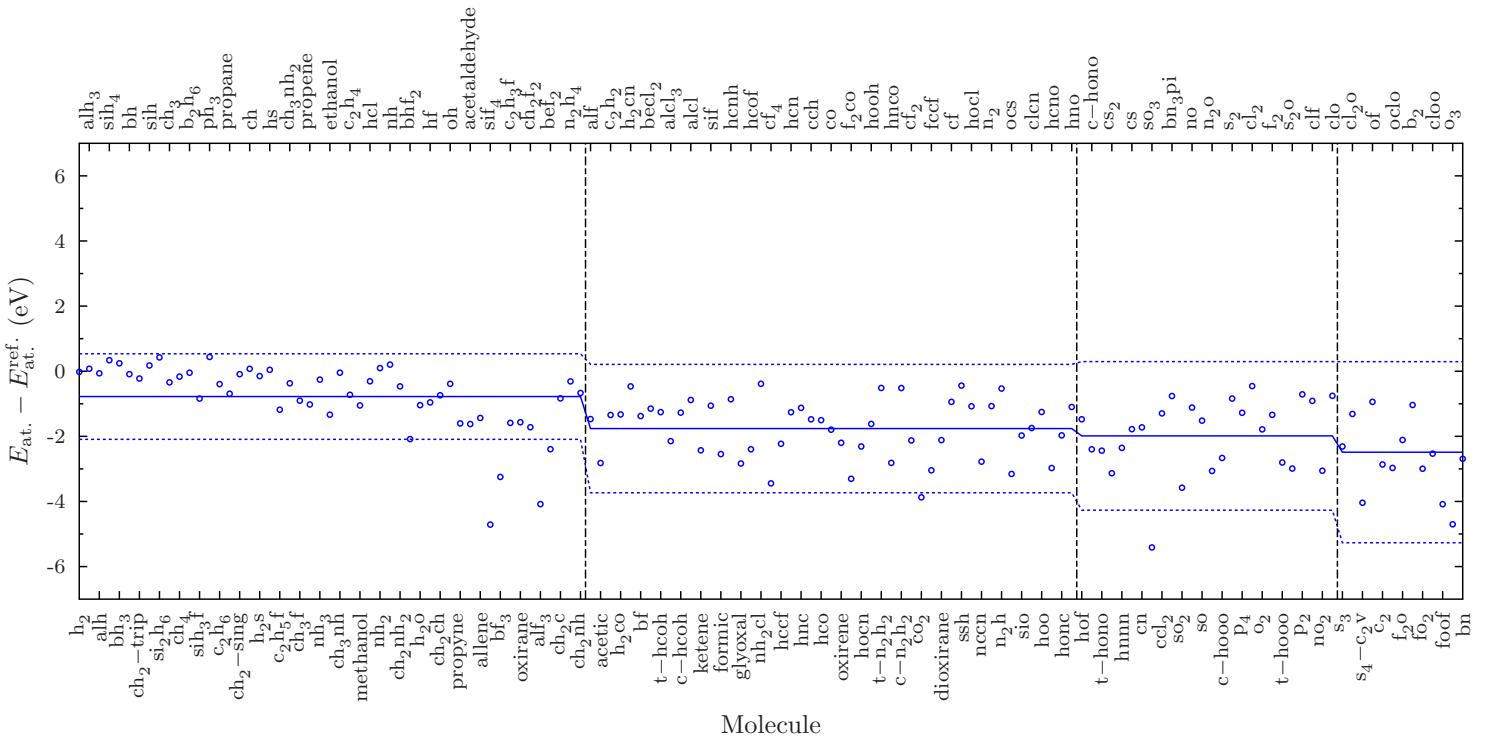


Figure 23: B3LYP PZ-RSIC results.

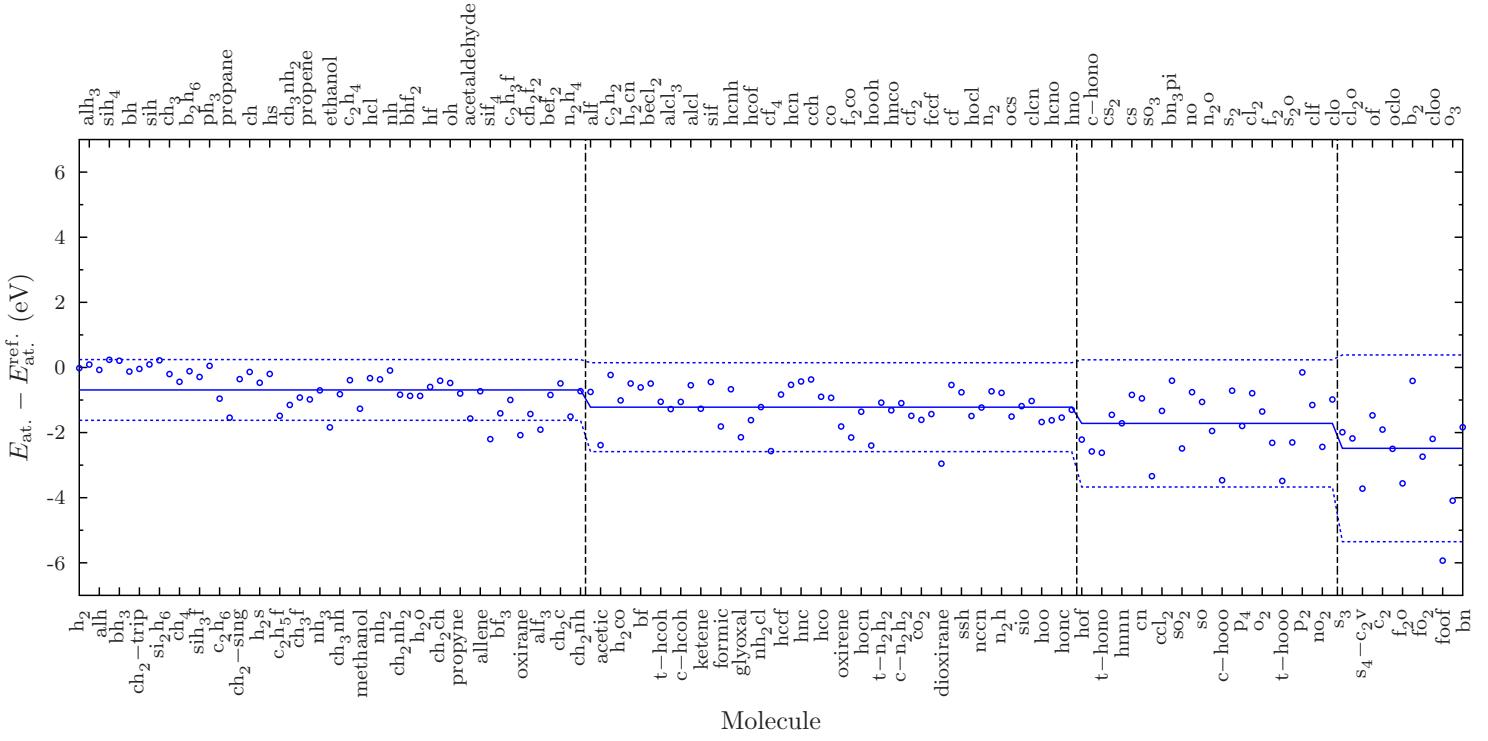


Figure 24: B3LYP PZ-SIC results.

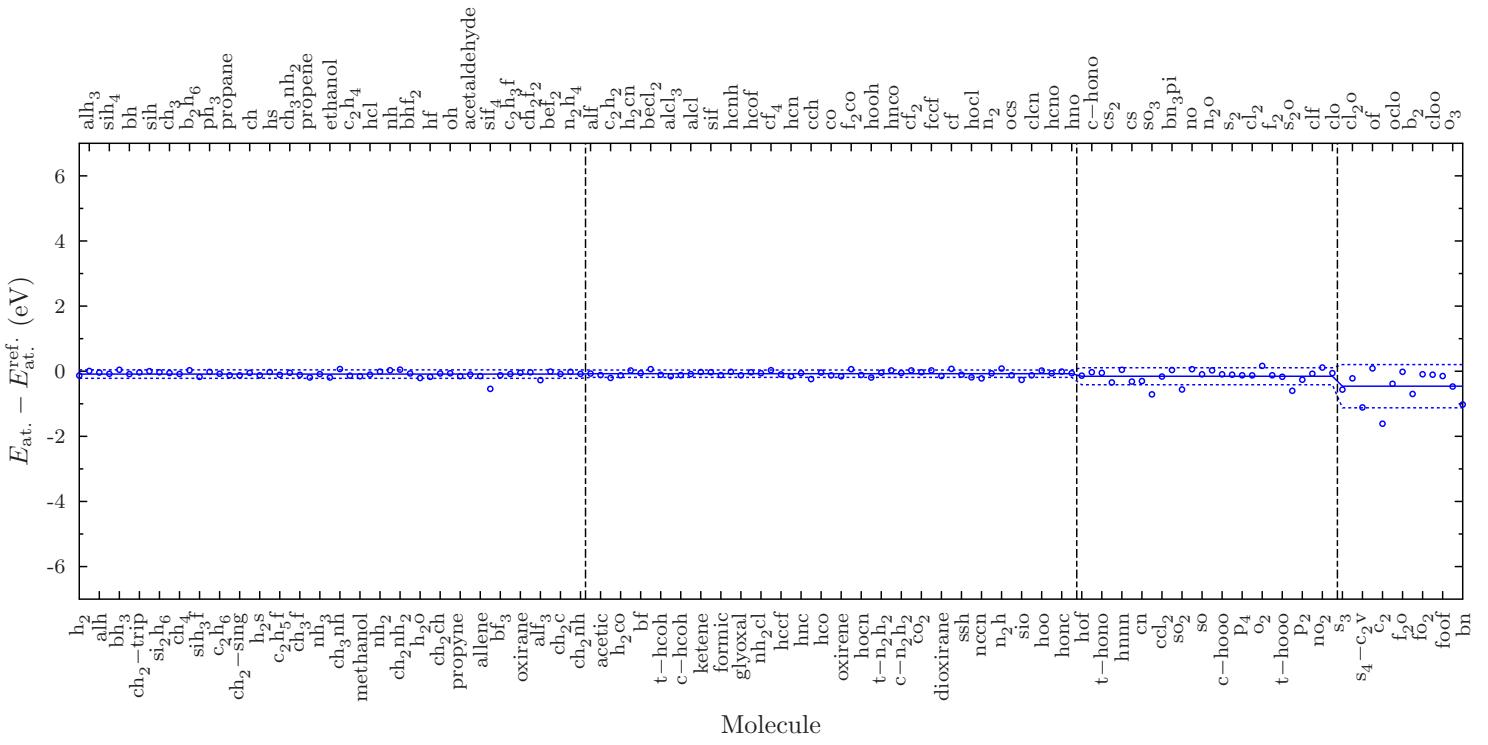


Figure 25:  $\omega$ B97X KS-DFT results.

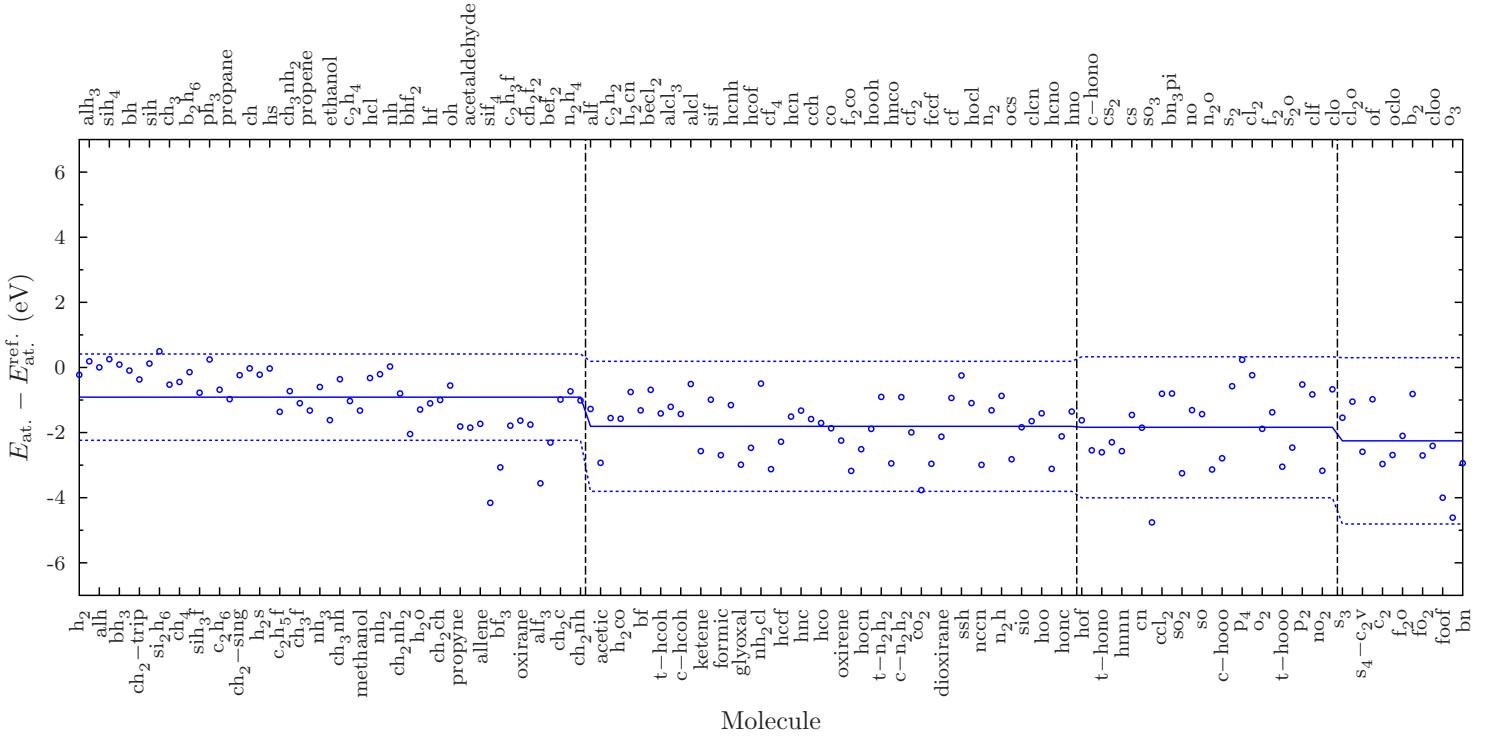


Figure 26:  $\omega$ B97X PZ-RSIC results.

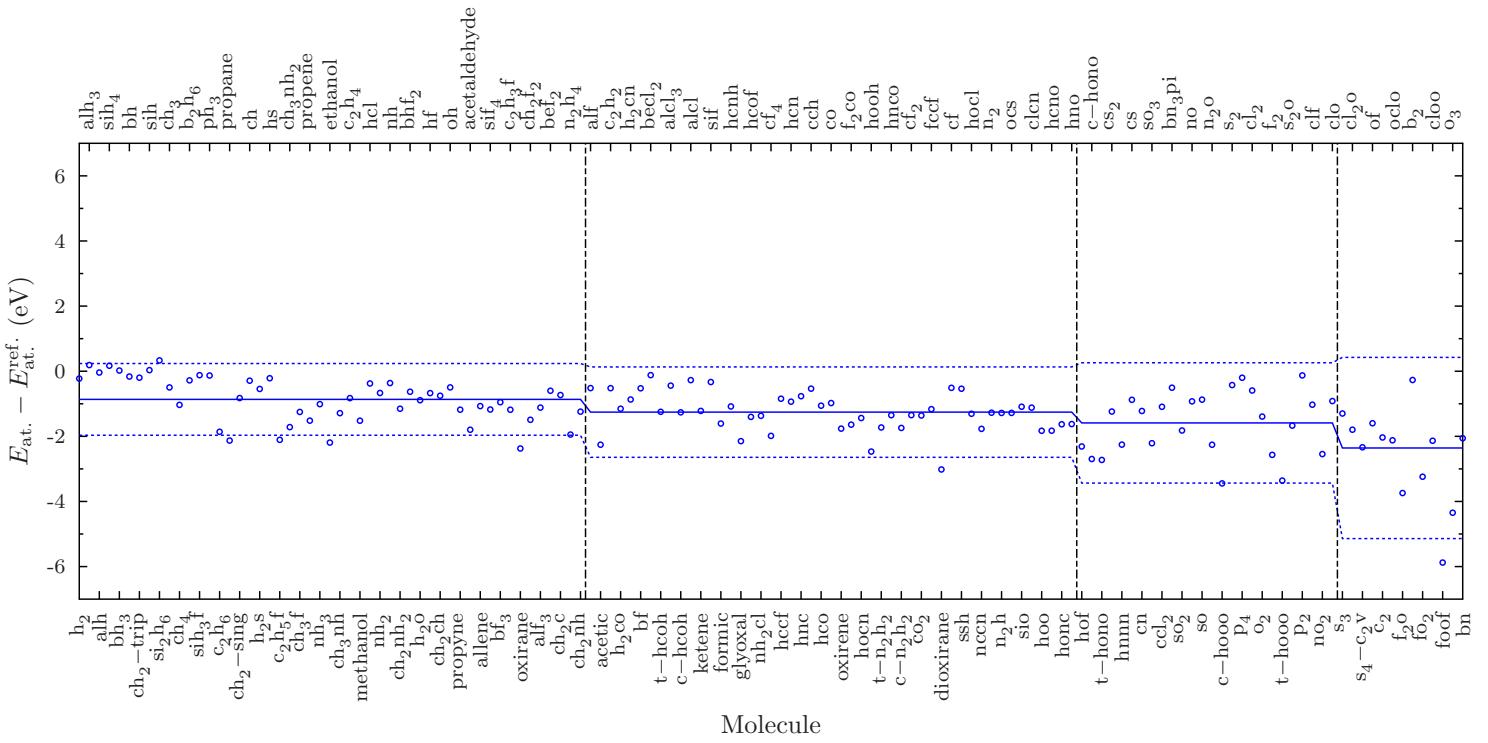


Figure 27:  $\omega$ B97X PZ-SIC results.

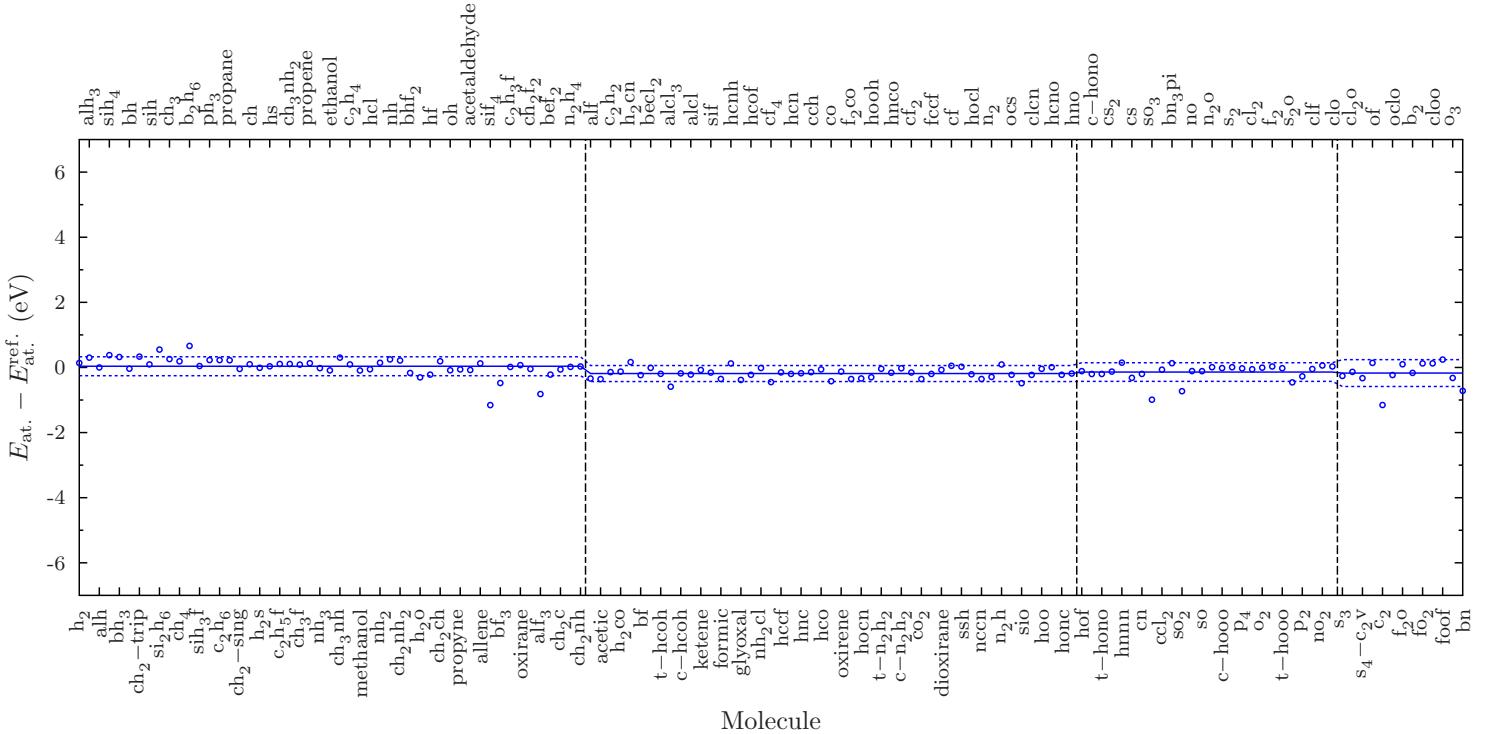


Figure 28: TPSSh KS-DFT results.

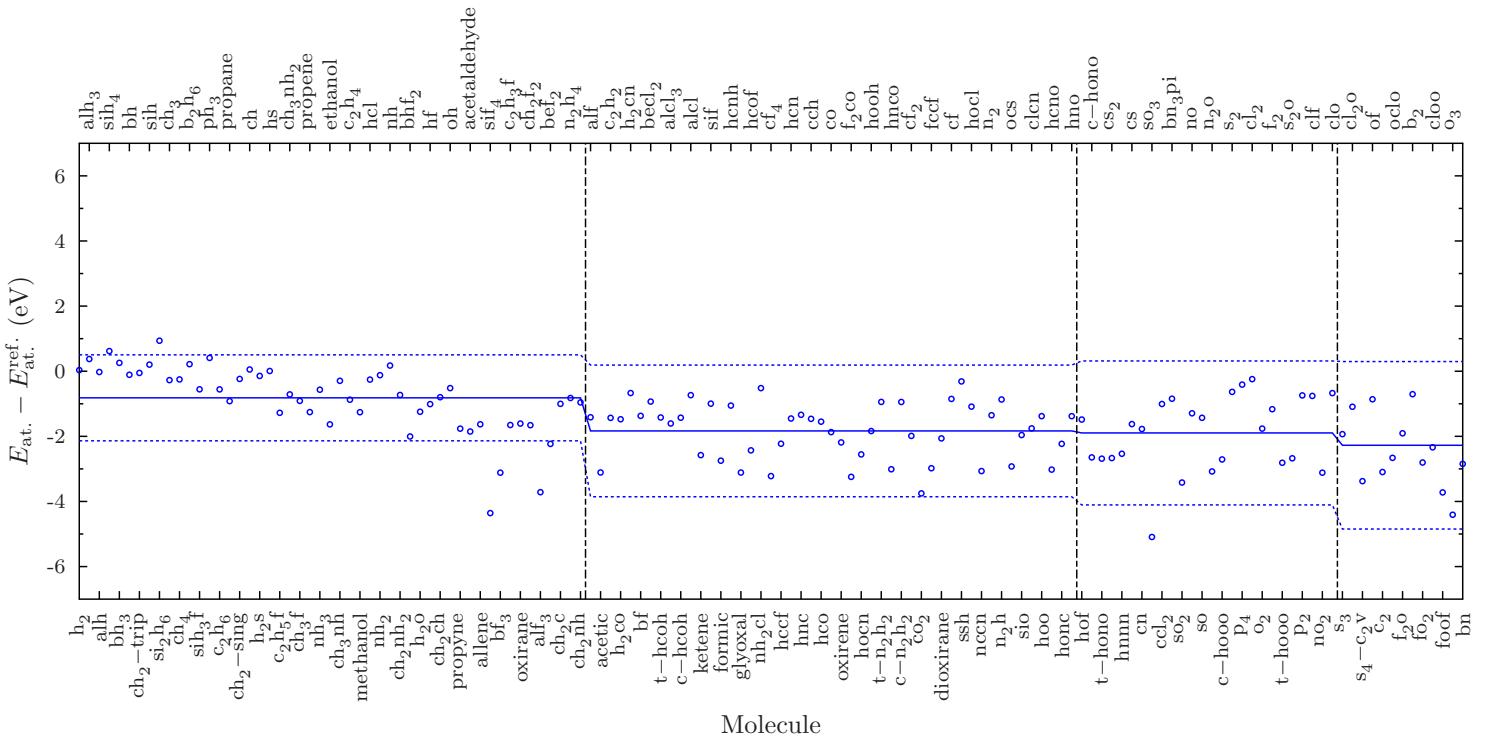


Figure 29: TPSSh PZ-RSIC results.

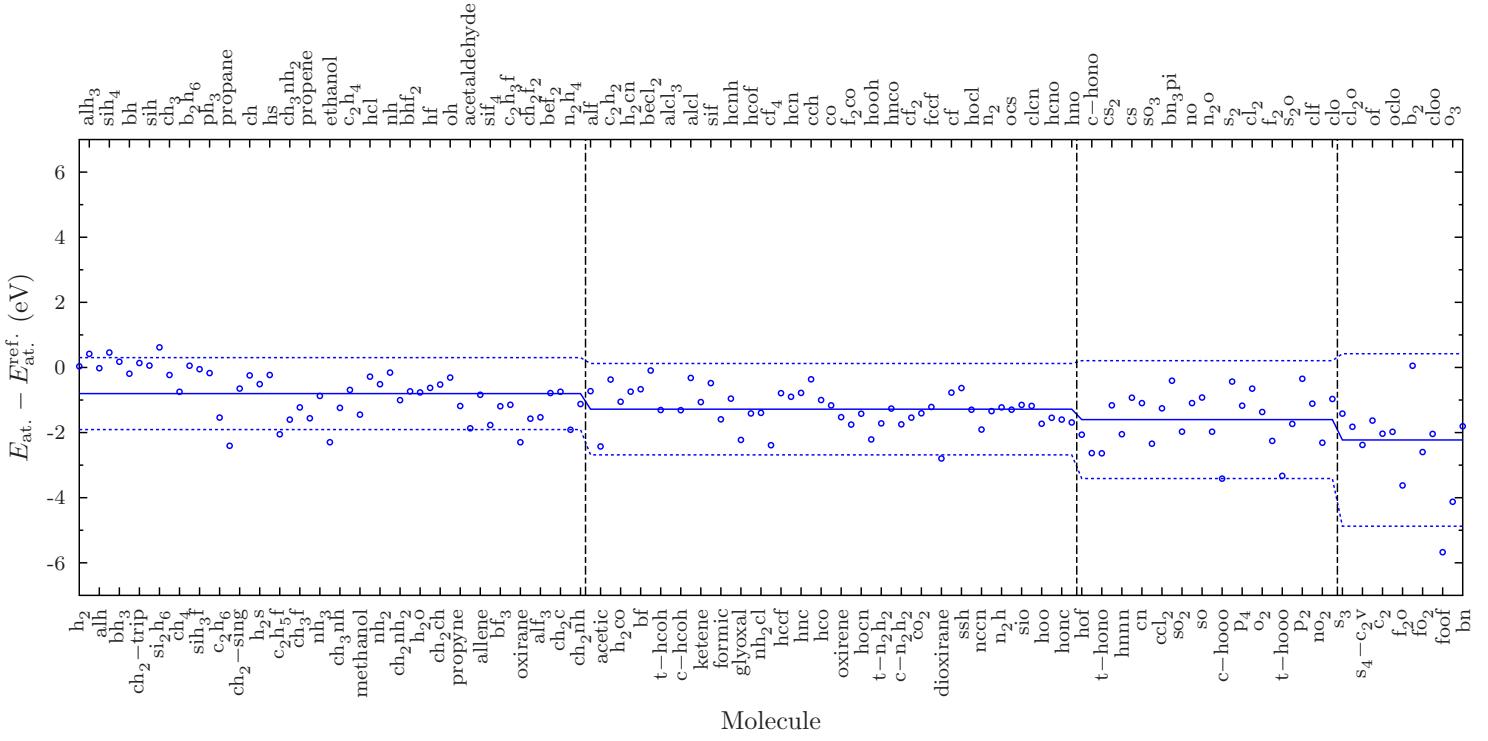


Figure 30: TPSSh PZ-SIC results.

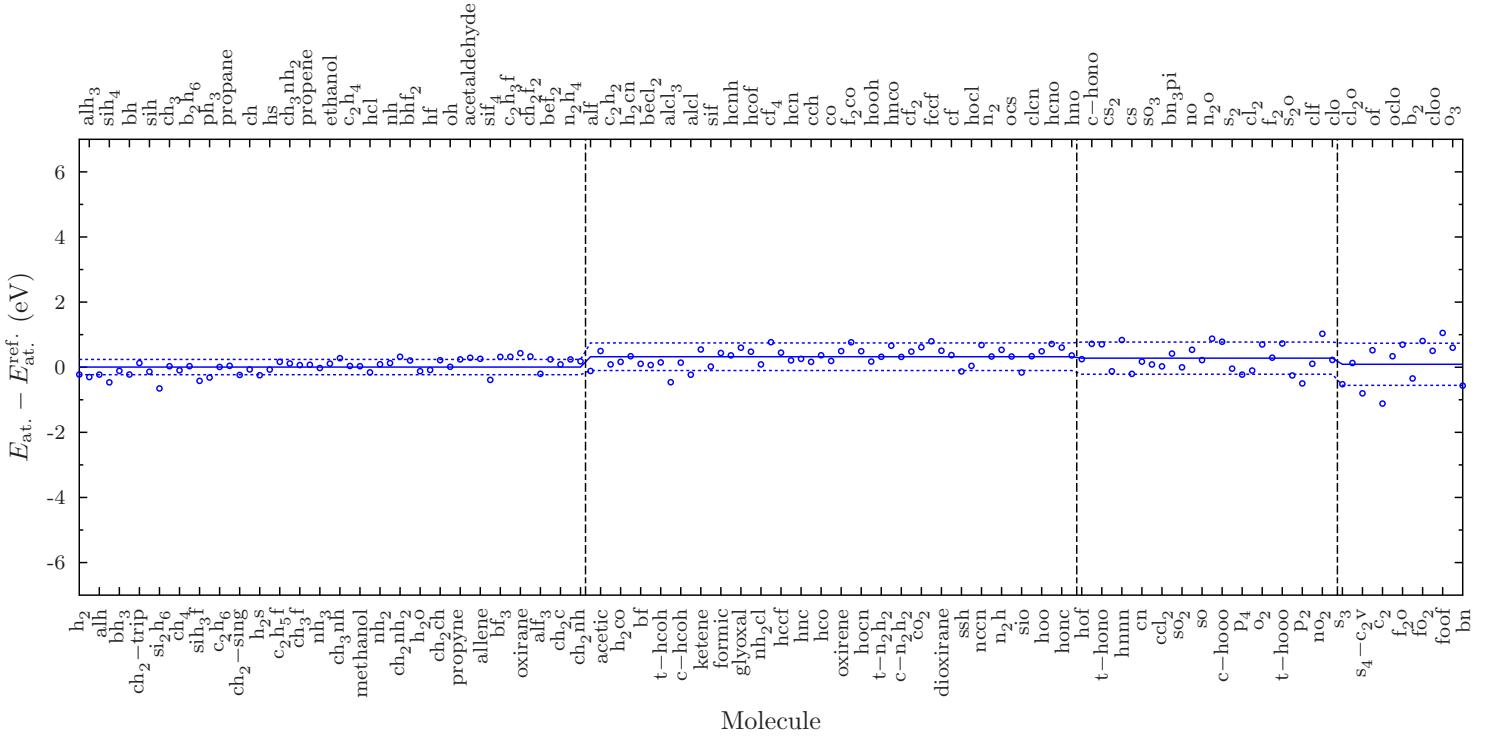


Figure 31: LRC- $\omega$ PBE KS-DFT results.

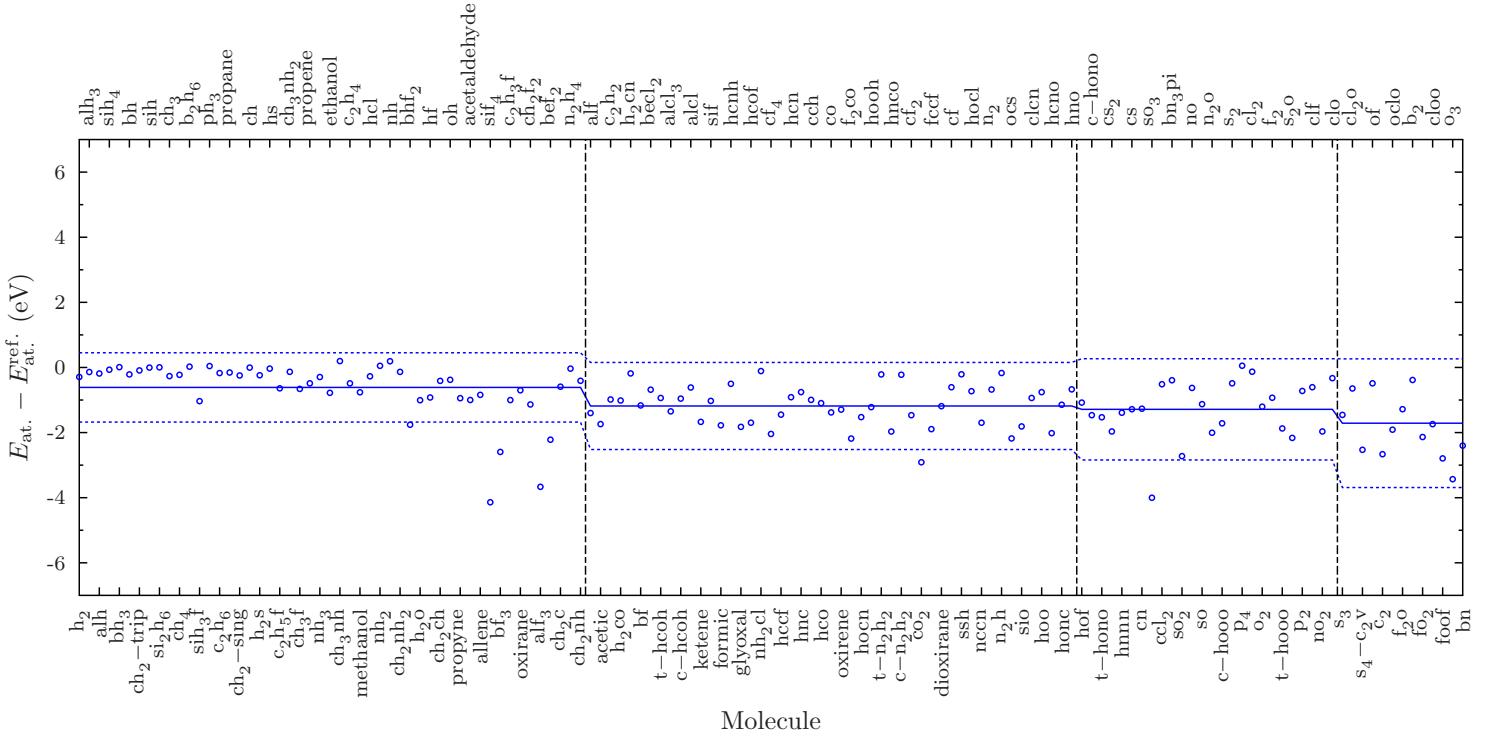


Figure 32: LRC- $\omega$ PBE PZ-RSIC results.

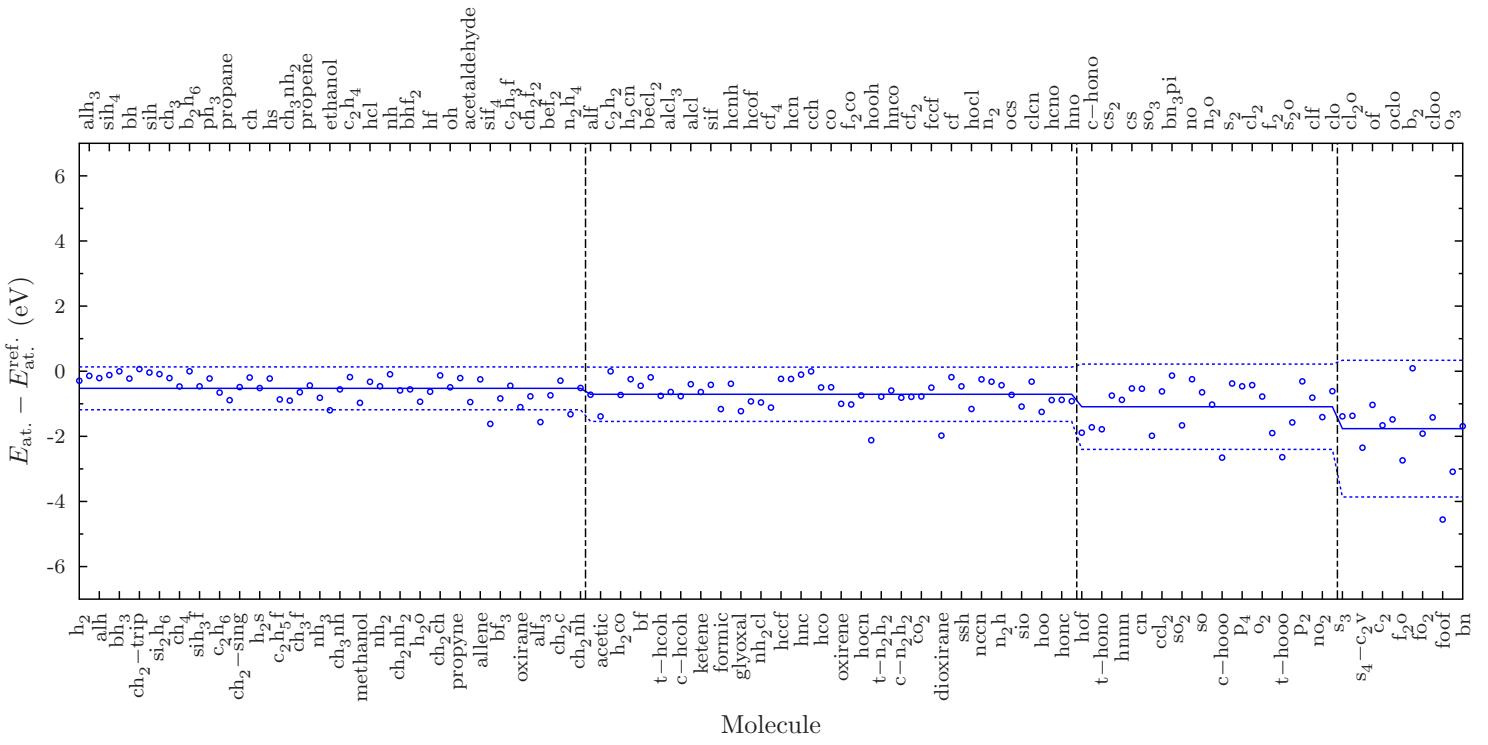


Figure 33: LRC- $\omega$ PBE PZ-SIC results.

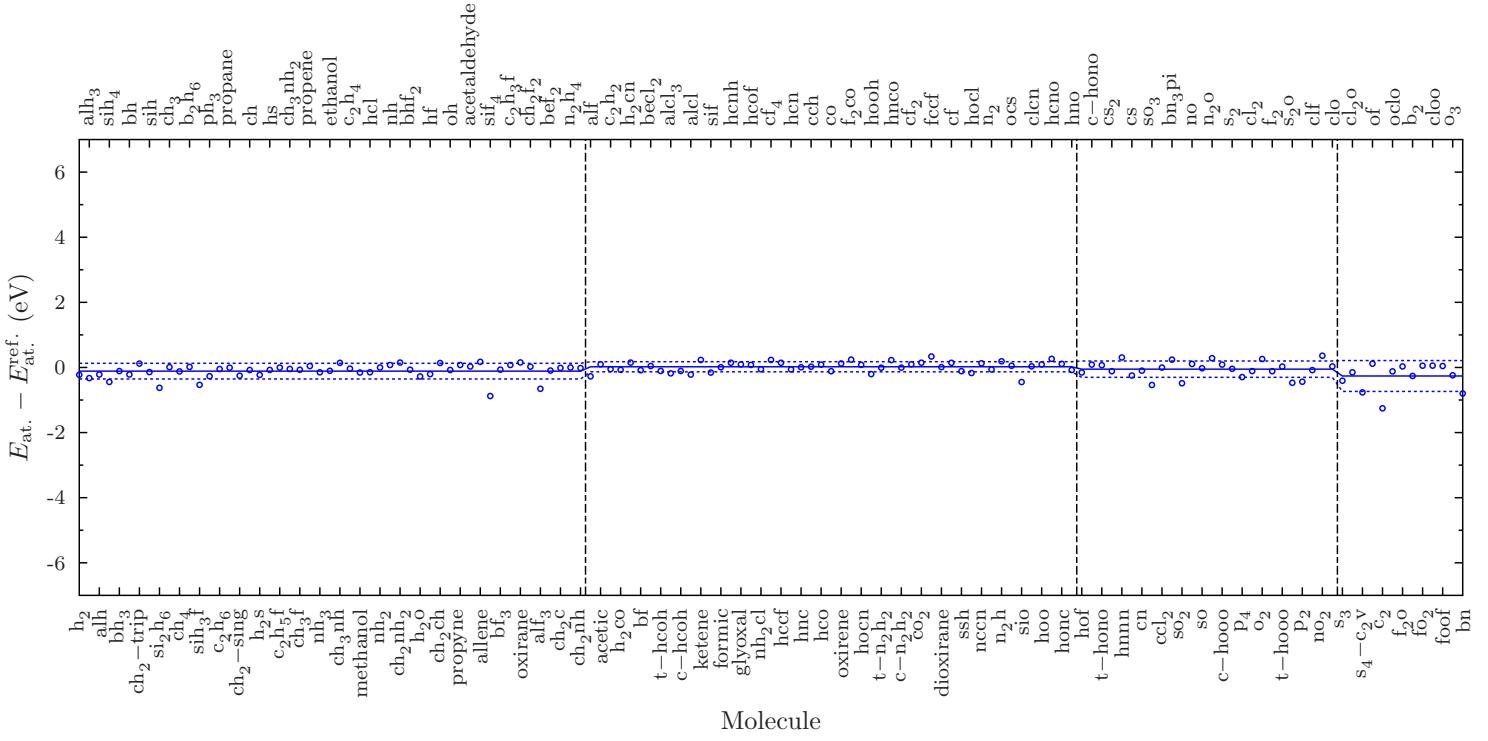


Figure 34: LRC- $\omega$ PBEh KS-DFT results.

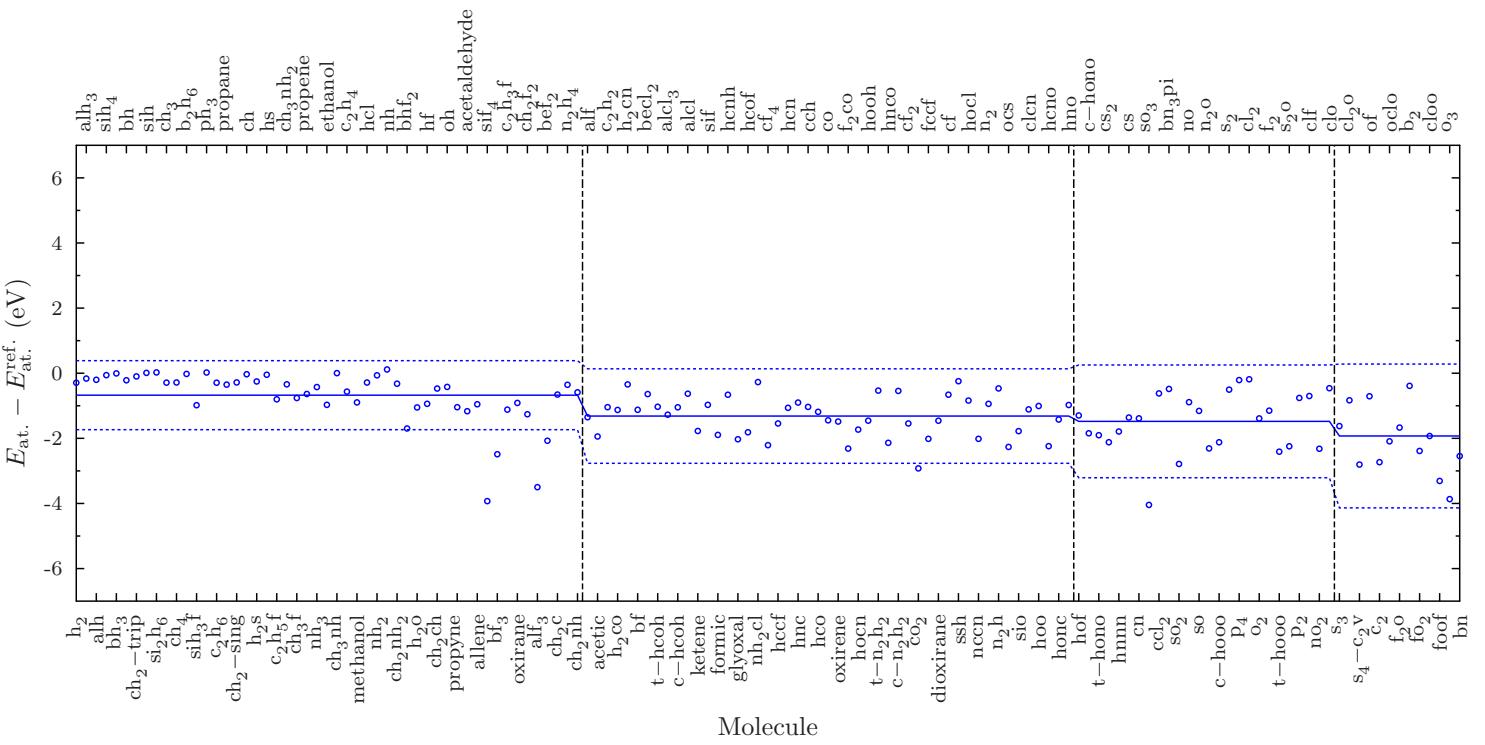


Figure 35: LRC- $\omega$ PBEh PZ-RSIC results.

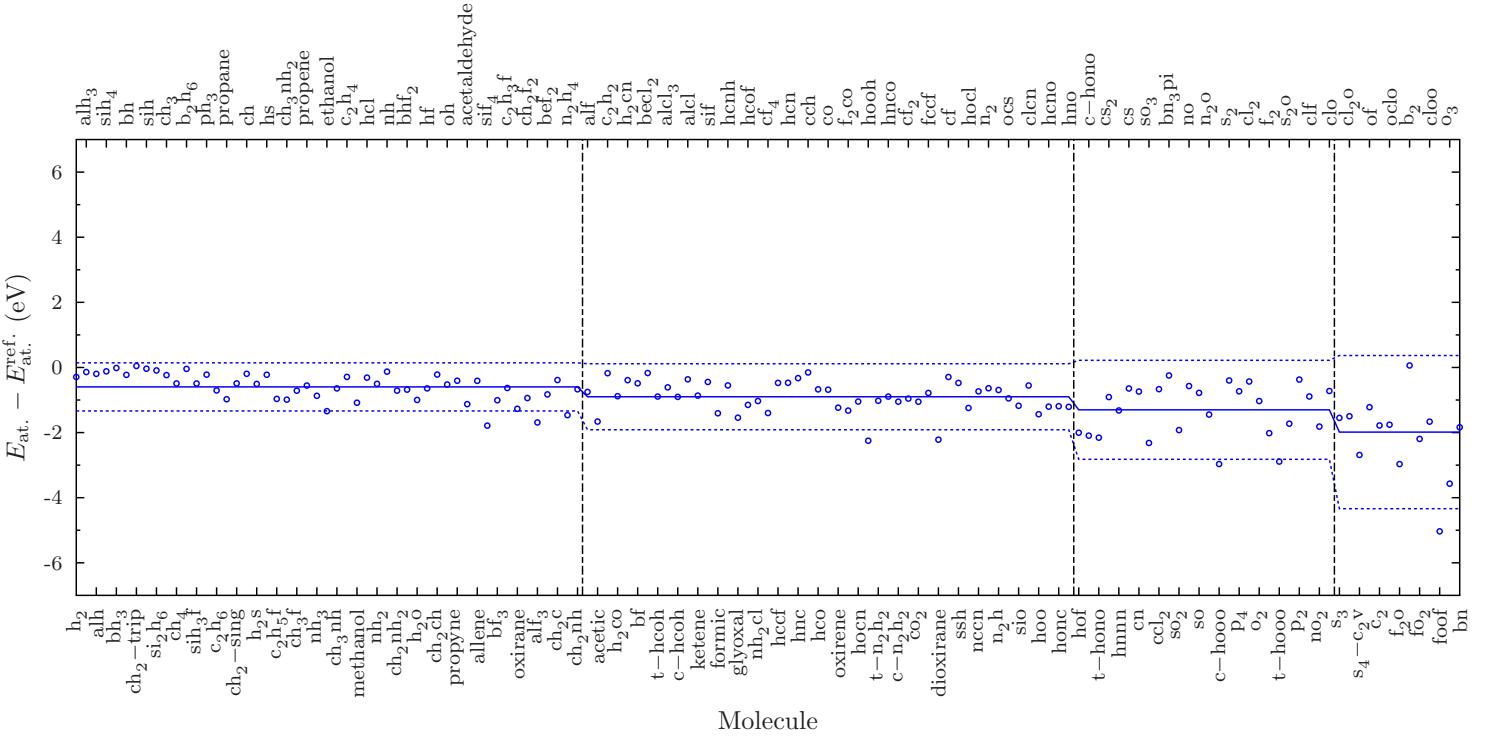


Figure 36: LRC- $\omega$ PBEh PZ-SIC results.