

Computational Analysis of Carbon Nano-Onions and Fullerenes with Point Defects: Stability and Electronic Properties

Supplementary material

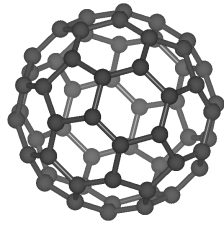
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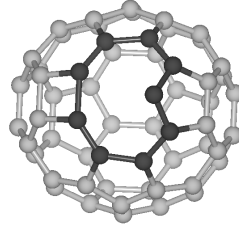
*Correspondence author: mmarquez@instec.cu

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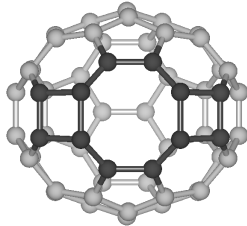
1 Optimized Structures with Point Defects.



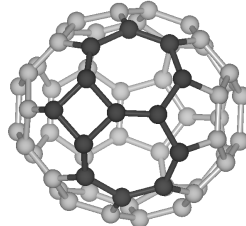
1.1. C_{60}



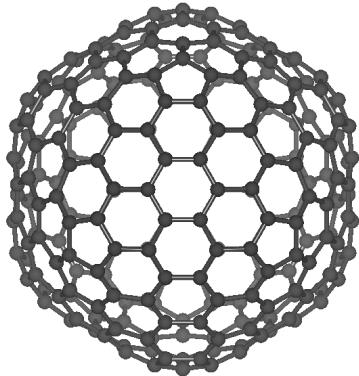
1.2. C_{60} SV p



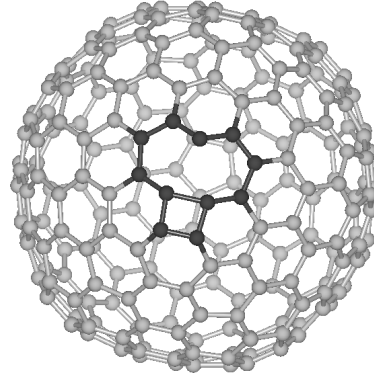
1.3. C_{60} DV p...p



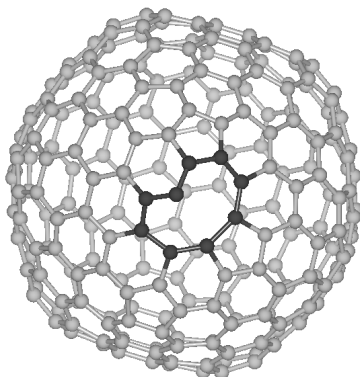
1.4. C_{60} SW p-p



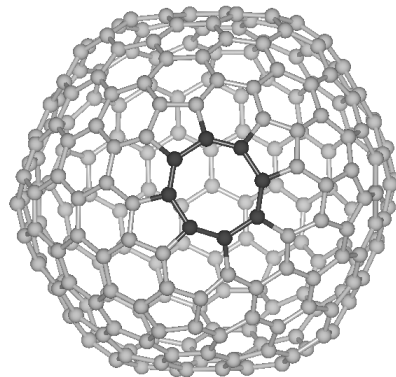
1.5. C_{240}



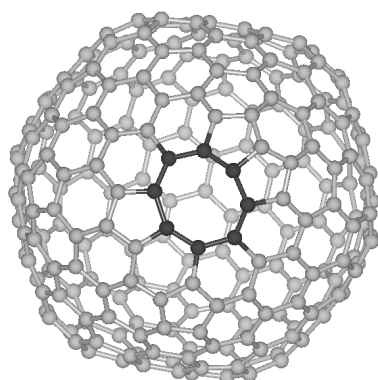
1.6. C_{240} SV p



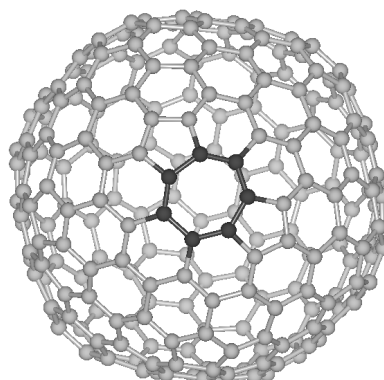
1.7. C_{240} SV h



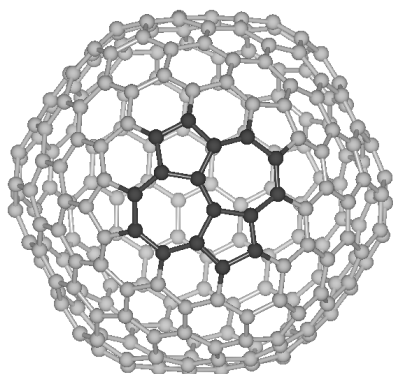
1.8. C_{240} DV h-h



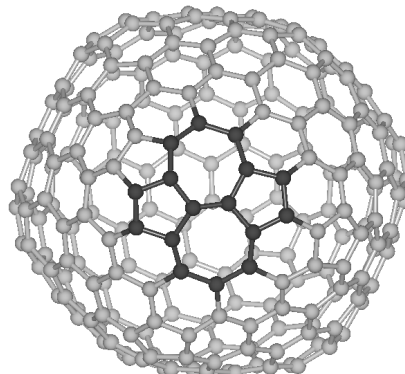
1.9. C_{240} DV hp-h



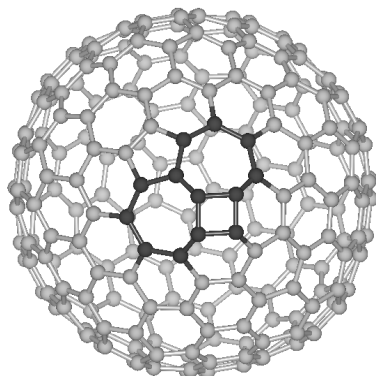
1.10. C_{240} DV p-p



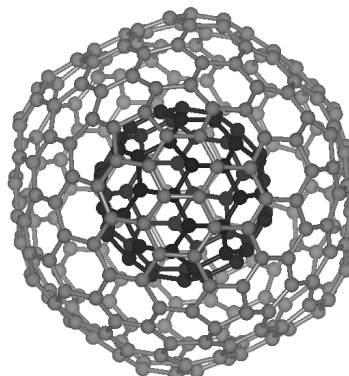
1.11. C_{240} SW h-h



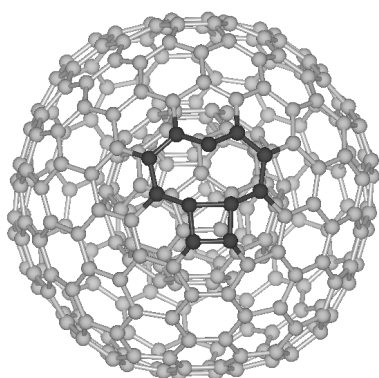
1.12. C_{240} SW hp-h



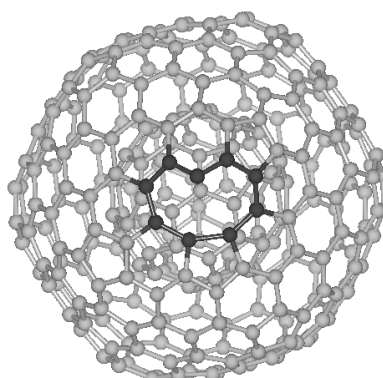
1.13. C_{240} SW p-p



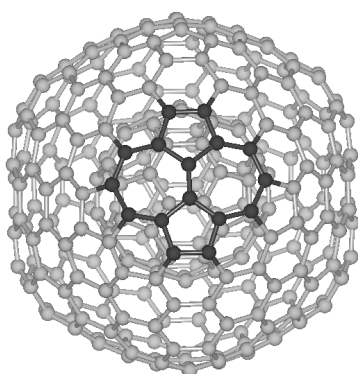
1.14. $C_{60}@C_{240}$



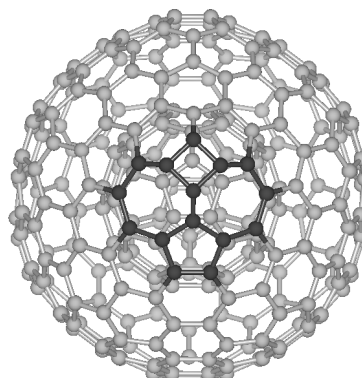
1.15. C₆₀@C₂₄₀ SV p



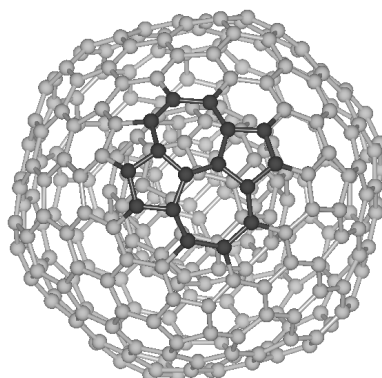
1.16. C₆₀@C₂₄₀ SV h



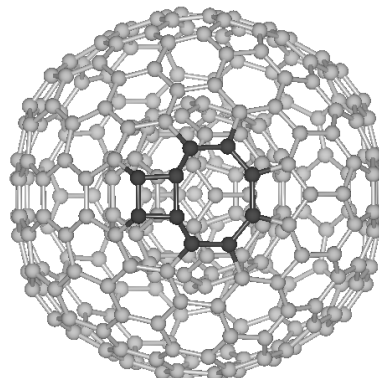
1.17. C₆₀@C₂₄₀ SW h-h



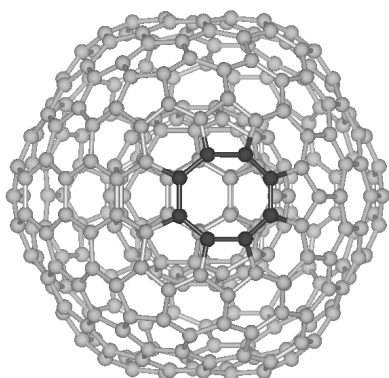
1.18. C₆₀@C₂₄₀ SW p-p



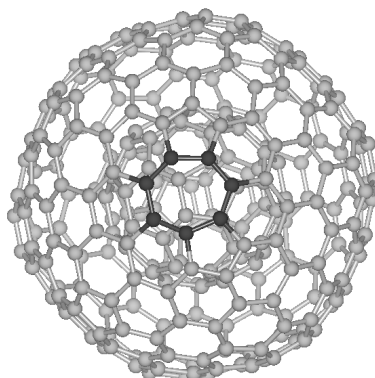
1.19. C₆₀@C₂₄₀ DV hp-h



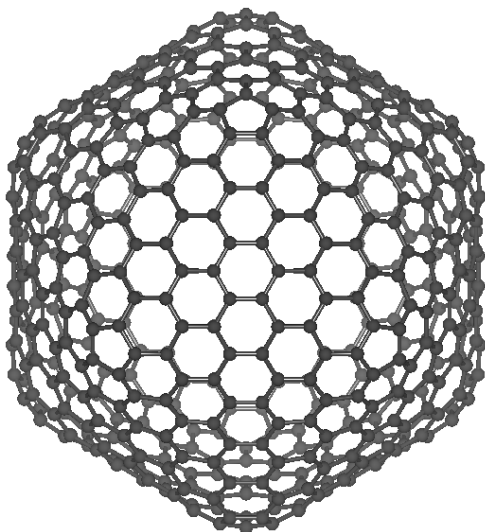
1.20. C₆₀@C₂₄₀ DV p-hp



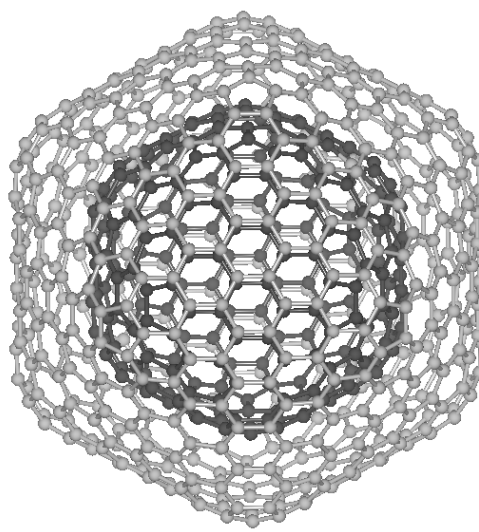
1.21. $C_{60}@C_{240}$ DV h-h



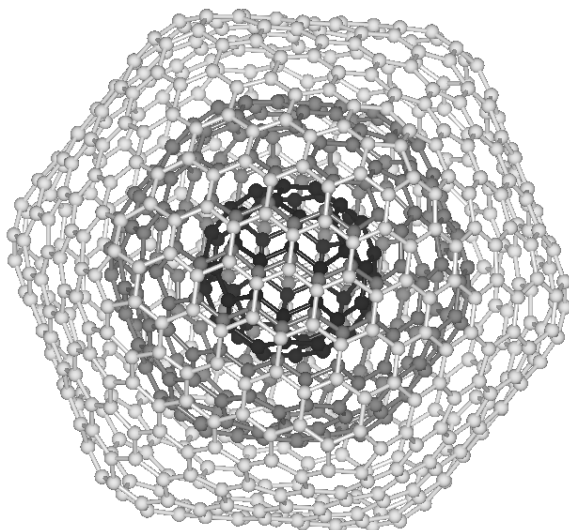
1.22. $C_{60}@C_{240}$ DV p-p



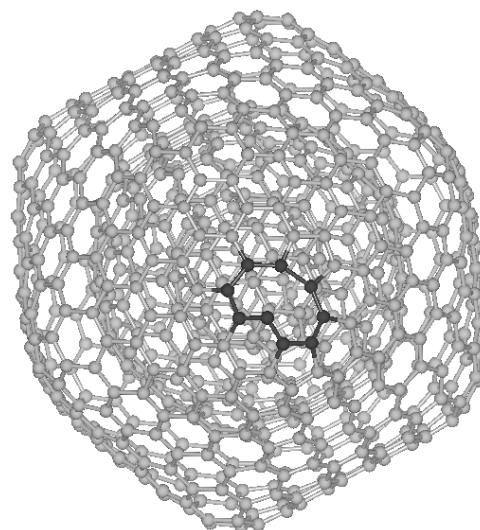
1.23. C_{540}



1.24. $C_{240}@C_{540}$



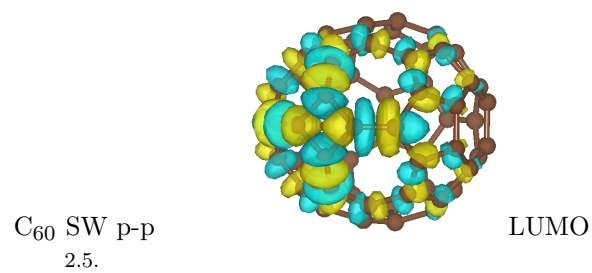
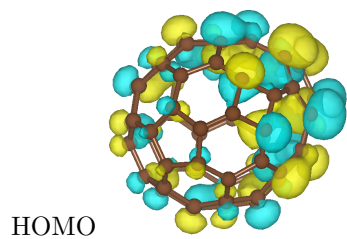
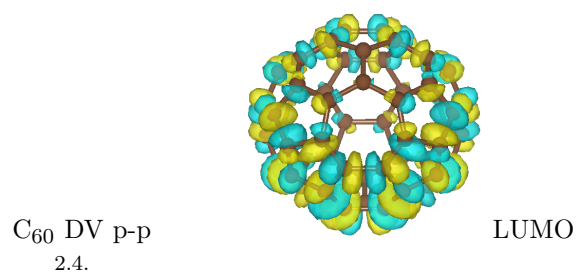
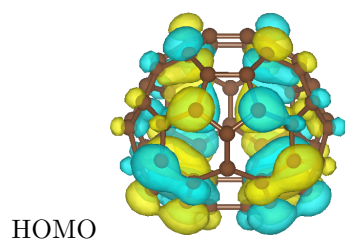
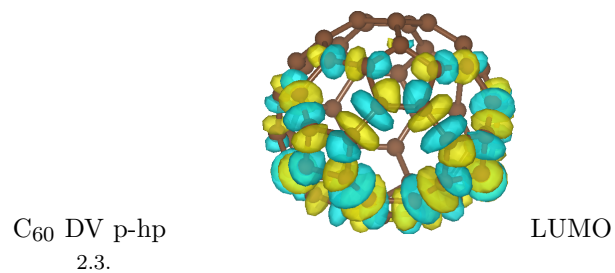
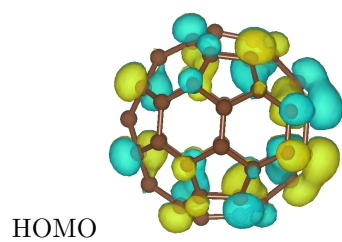
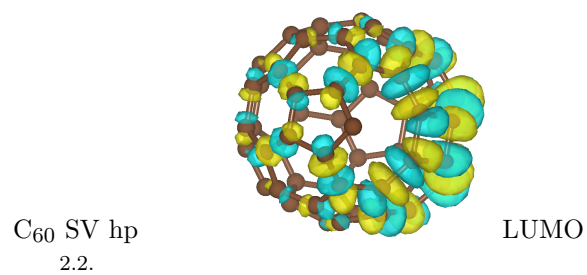
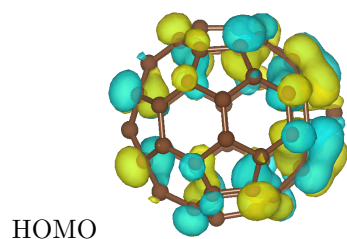
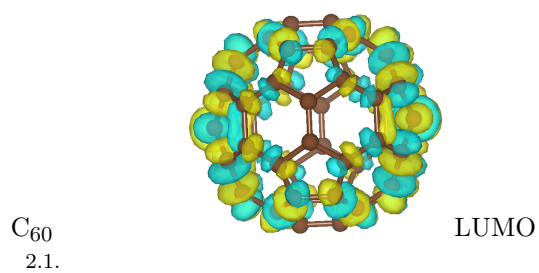
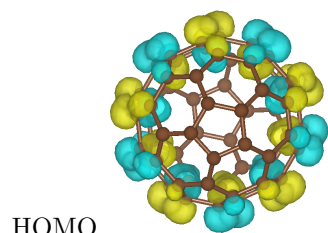
1.25. $C_{60}@C_{240}@C_{540}$

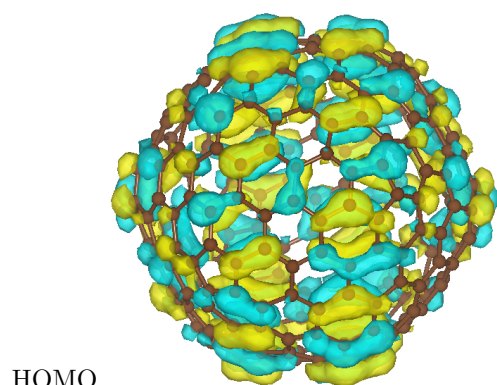


1.26. $C_{60}@C_{240}@C_{540}$ SV h

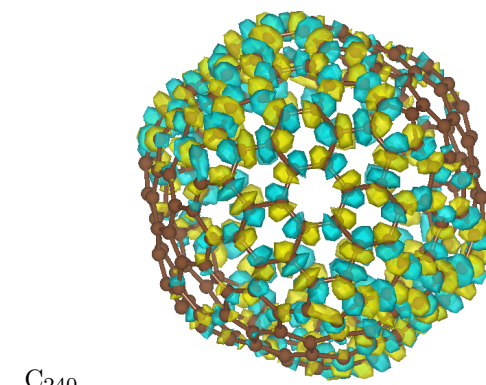
Figure 1: Optimized Structures with Point Defects.

2 HOMO and LUMO orbitals.



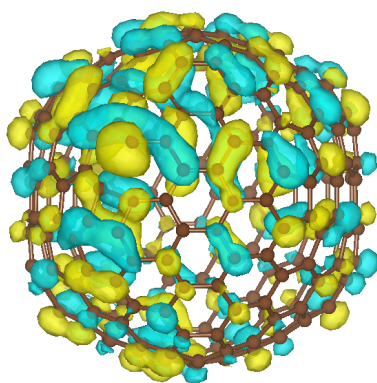


HOMO



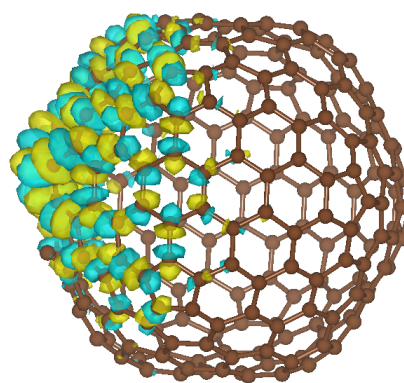
LUMO

C_{240}
2.6.

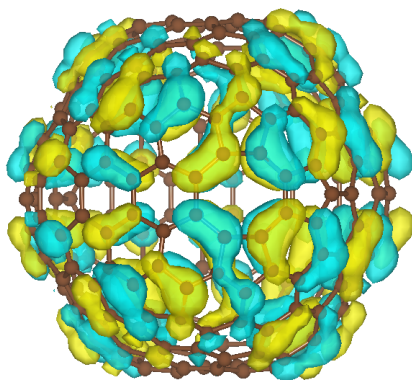


HOMO

C_{240} SV p
2.7.

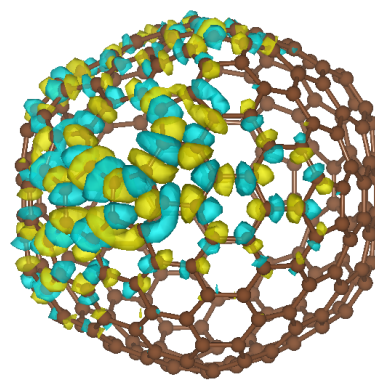


LUMO

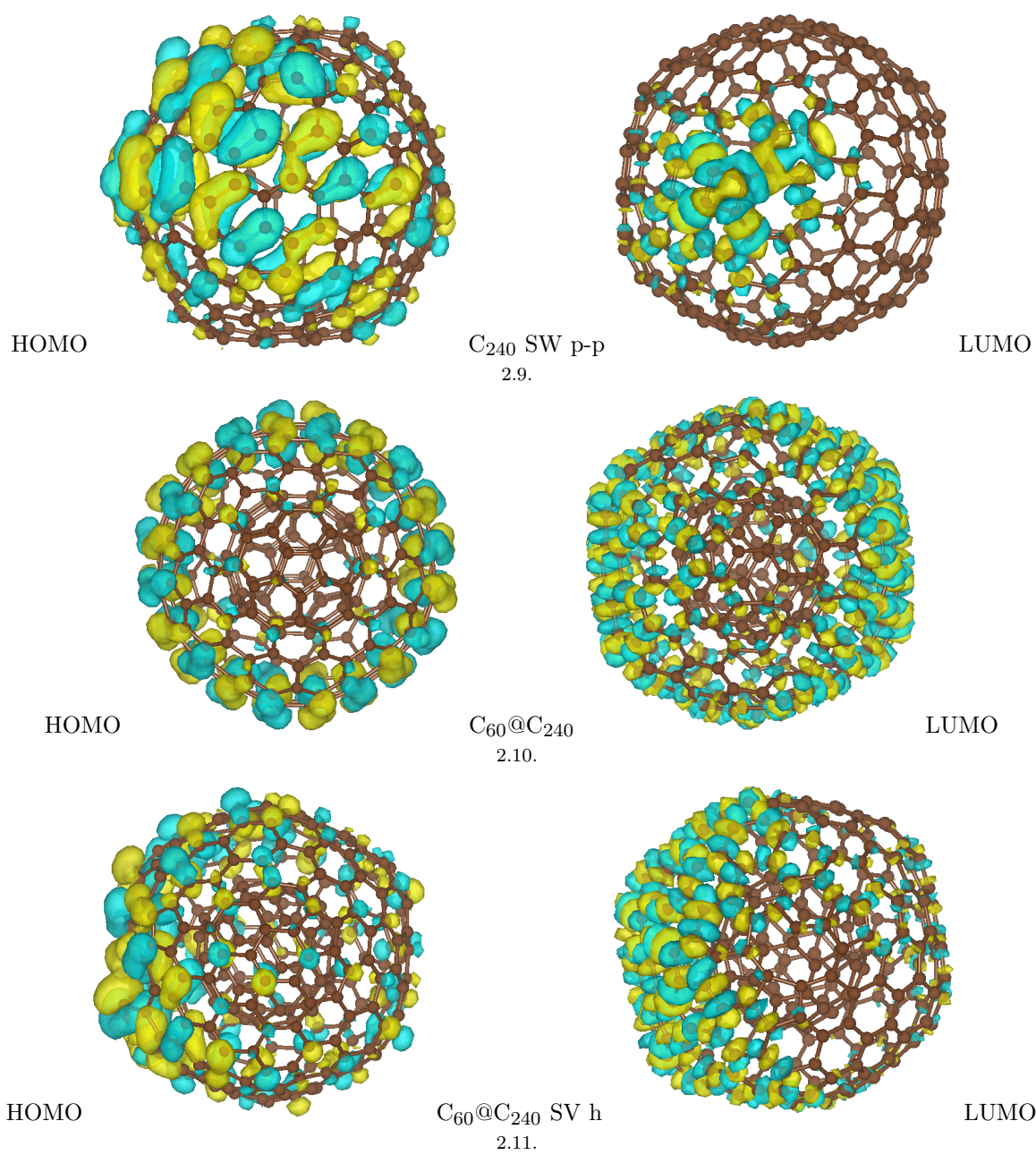


HOMO

C_{240} DV h-h
2.8.



LUMO



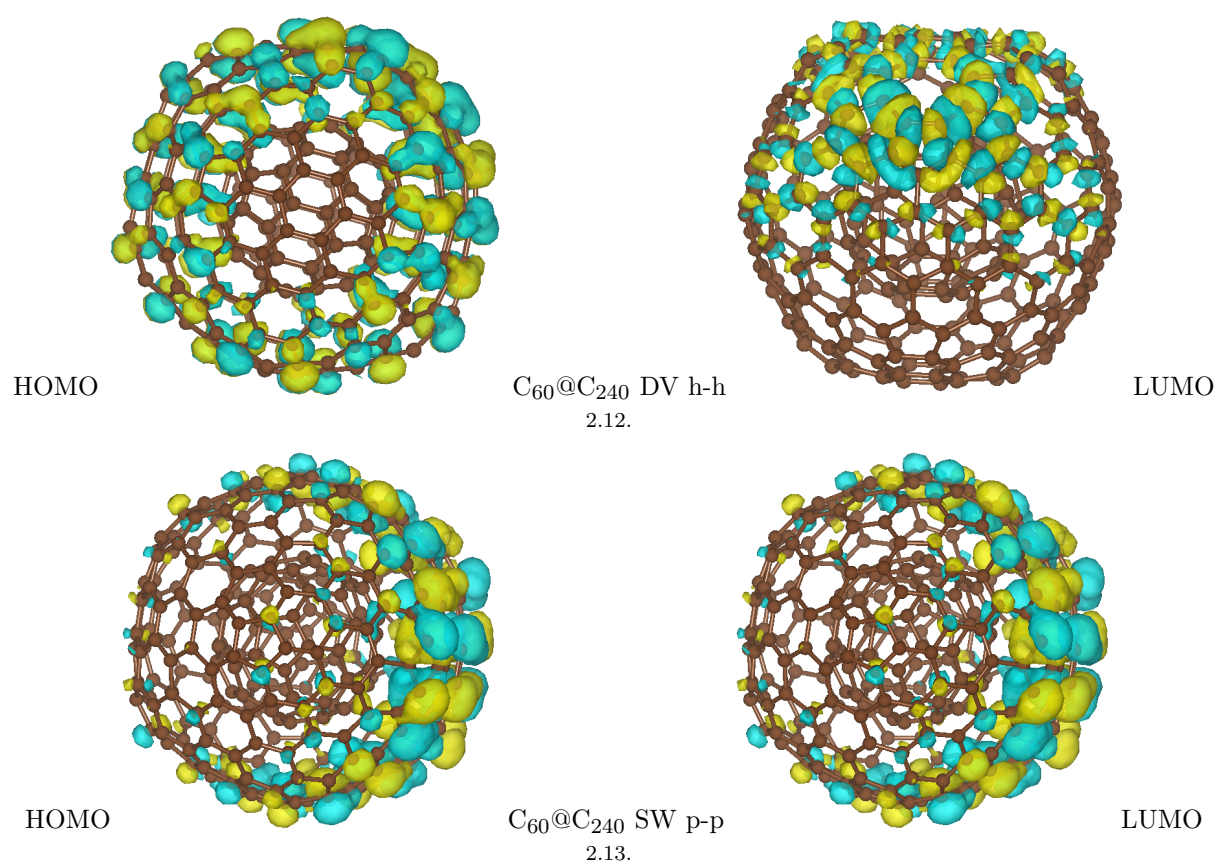
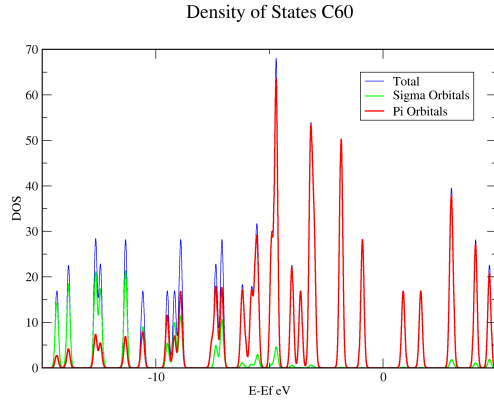
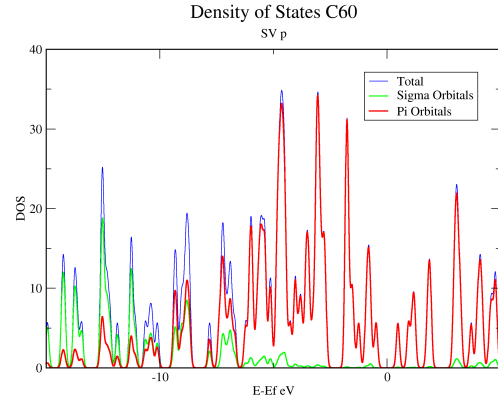


Figure 2: HOMO (left) and LUMO (right) of fullerene and CNOs, and some defects. Blue lobes represent negative charge density, yellow lobes represent positive charge density.

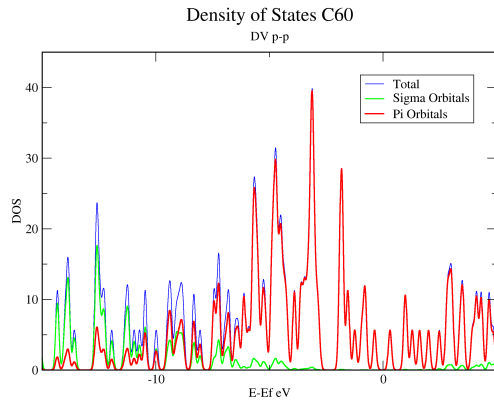
3 Density of States



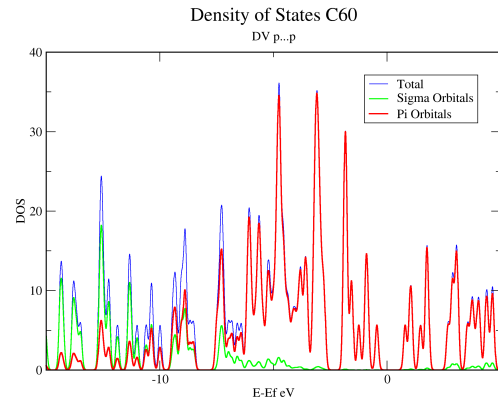
3.1. C₆₀



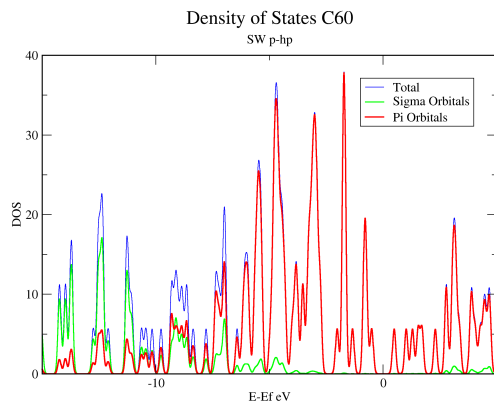
3.2. C₆₀ SV p



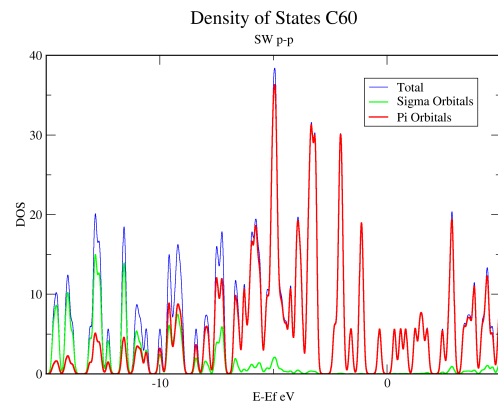
3.3. C₆₀ DV p-p



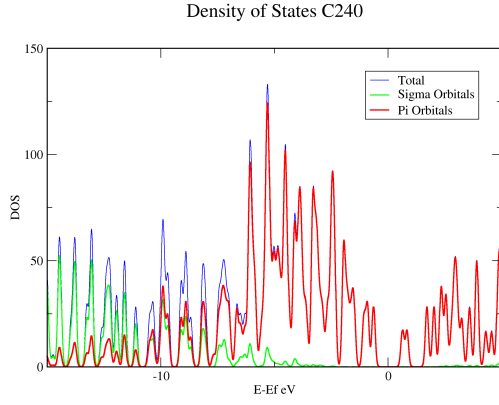
3.4. C₆₀ DV p...p



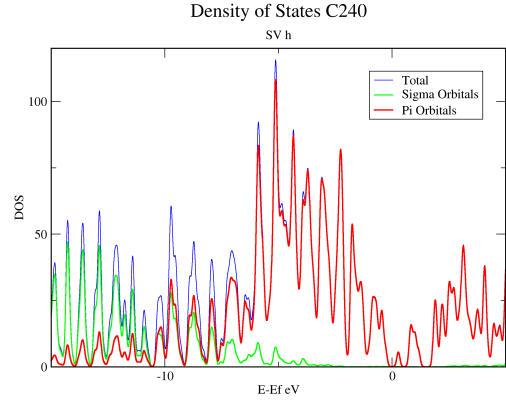
3.5. C₆₀ SW p-hp



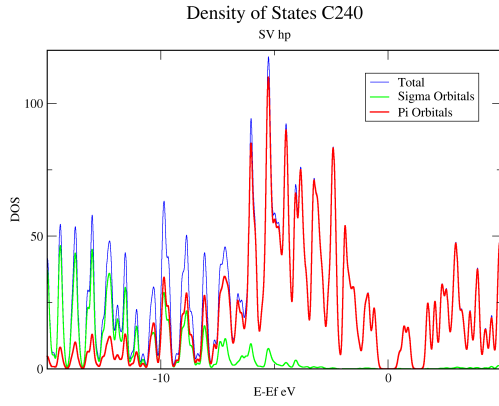
3.6. C₆₀ SW p-p



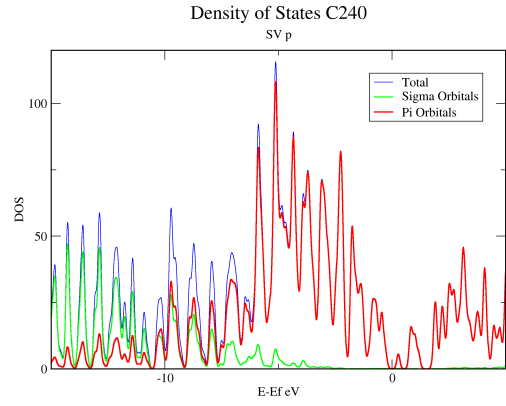
3.7. C₂₄₀



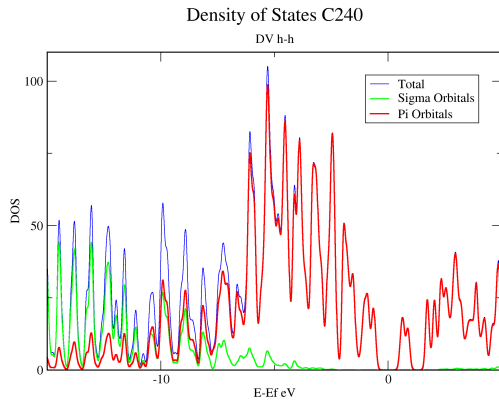
3.8. C₂₄₀ SV h



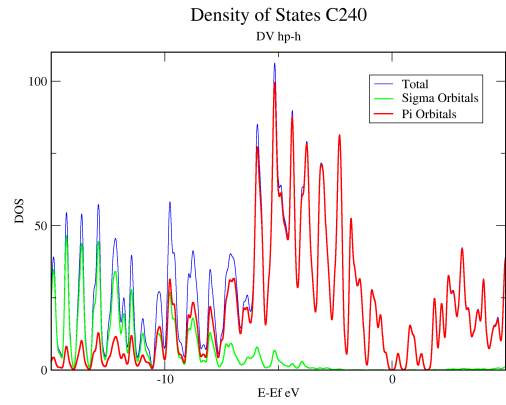
3.9. C₂₄₀ SV hp



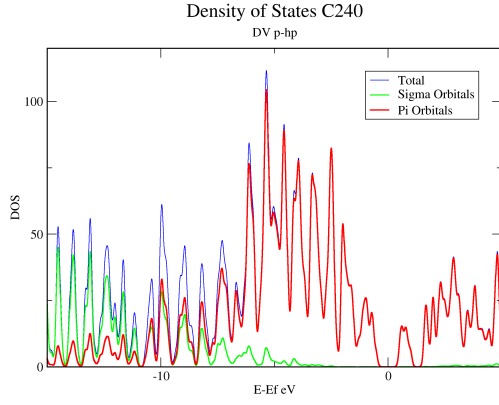
3.10. C₂₄₀ SV p



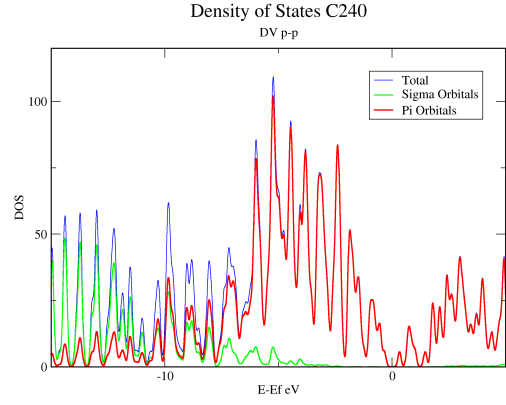
3.11. C₂₄₀ DV h-h



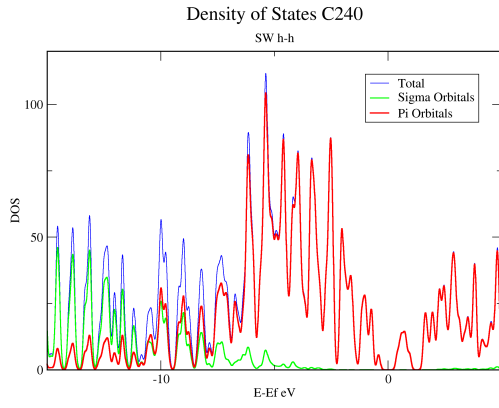
3.12. C₂₄₀ DV hp-h



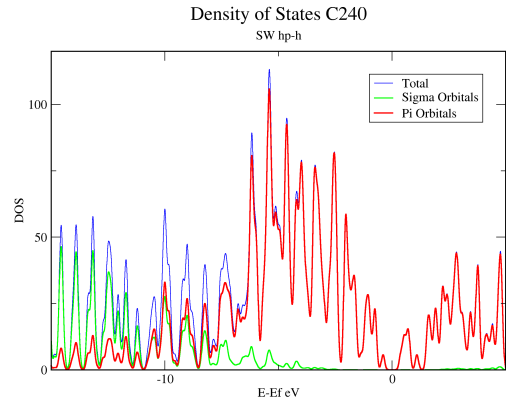
3.13. C₂₄₀ DV p-hp



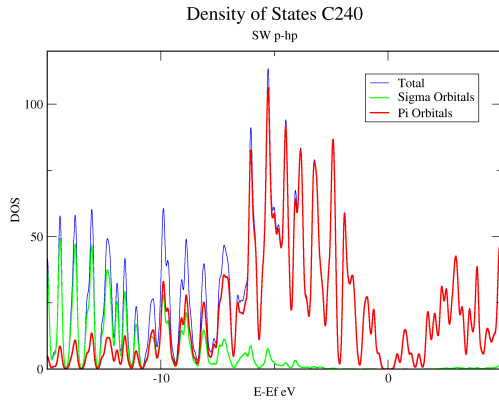
3.14. C₂₄₀ DV p-p



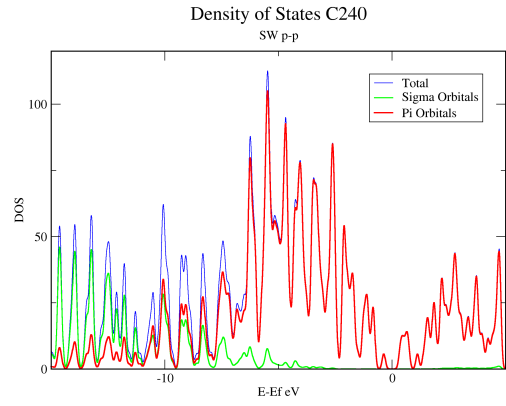
3.15. C₂₄₀ SW h-h



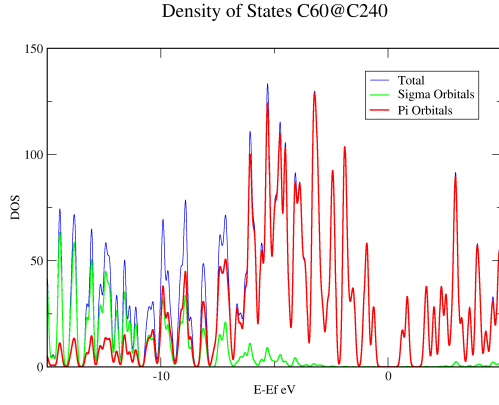
3.16. C₂₄₀ SW hp-h



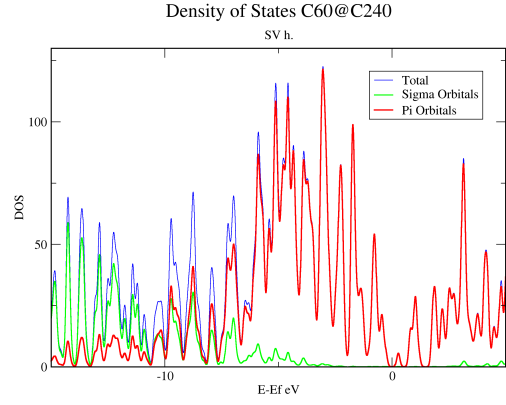
3.17. C₂₄₀ SW p-hp



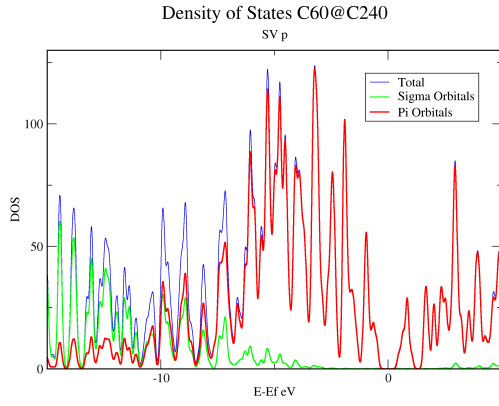
3.18. C₂₄₀ SW p-p



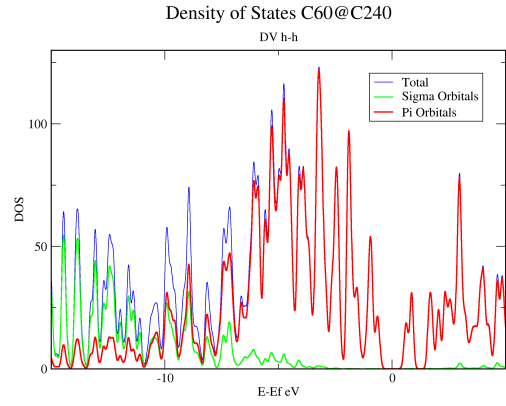
3.19. C₆₀@C₂₄₀



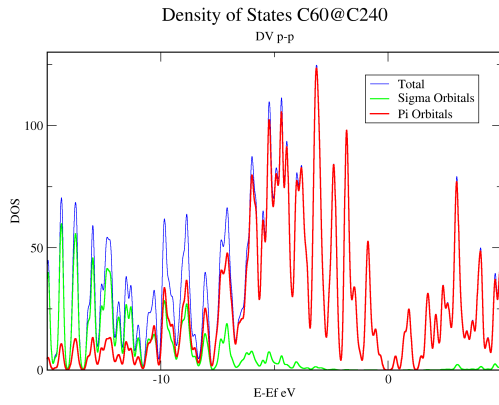
3.20. C₆₀@C₂₄₀ SV h



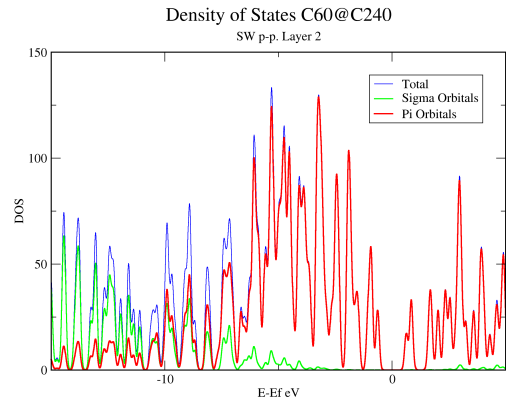
3.21. C₆₀@C₂₄₀ SV p



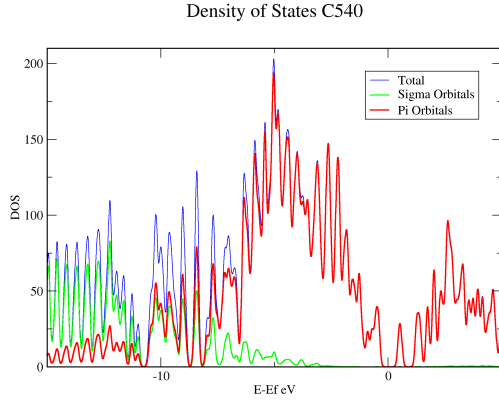
3.22. C₆₀@C₂₄₀ DV h-h



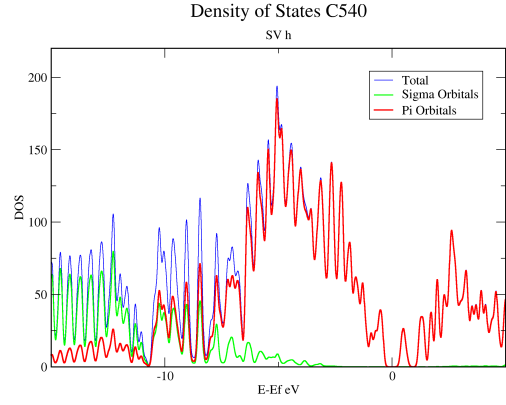
3.23. C₆₀@C₂₄₀ DV p-p



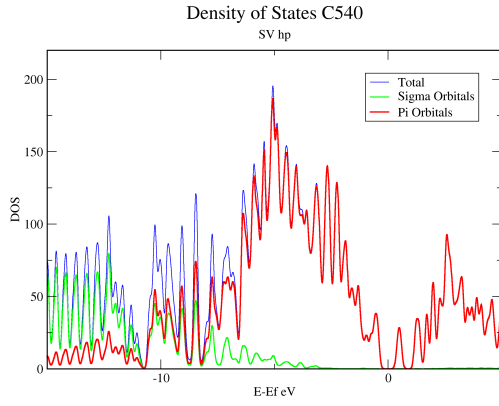
3.24. C₆₀@C₂₄₀ SW p-p



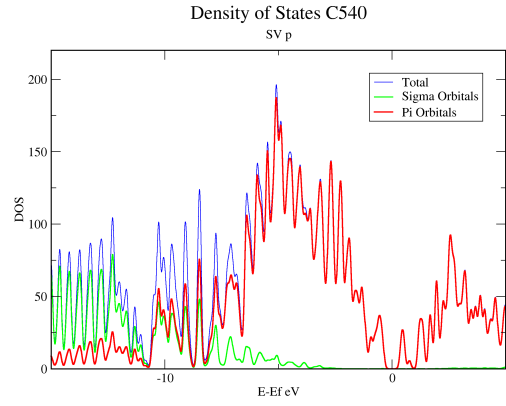
3.25. C₅₄₀



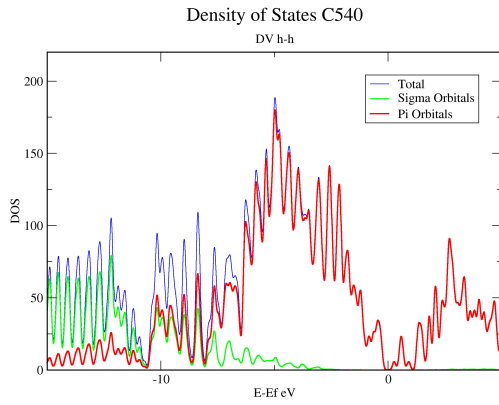
3.26. C₅₄₀ SV h



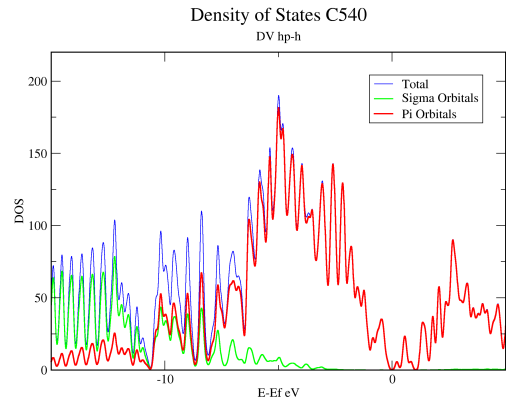
3.27. C₅₄₀ SV hp



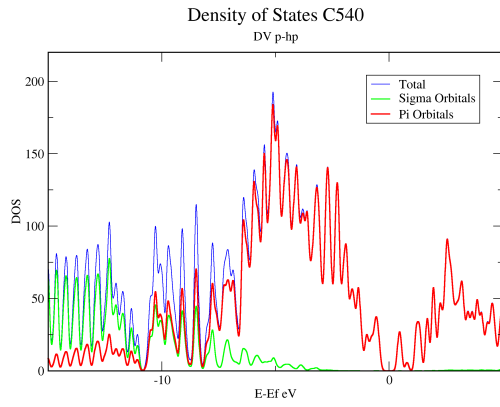
3.28. C₅₄₀ SV p



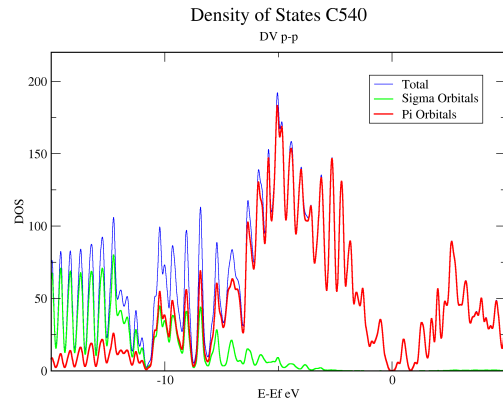
3.29. C₅₄₀ DV h-h



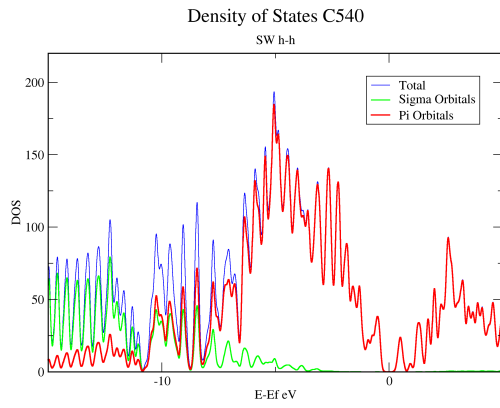
3.30. C₅₄₀ DV hp-h



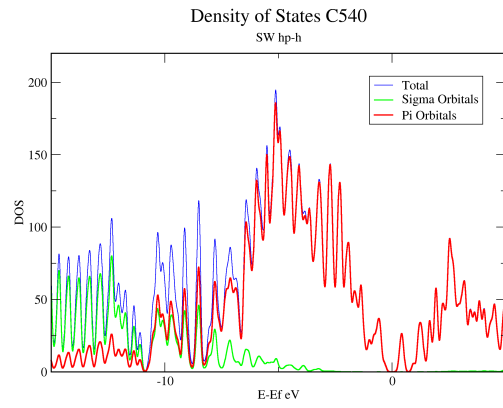
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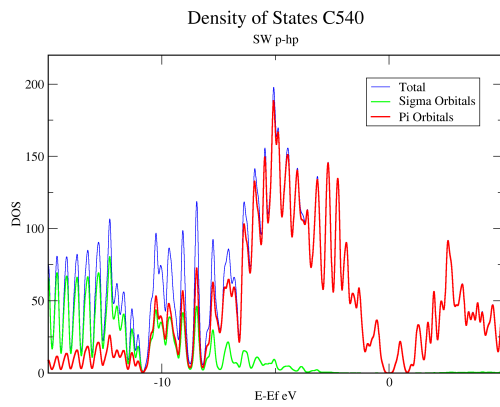
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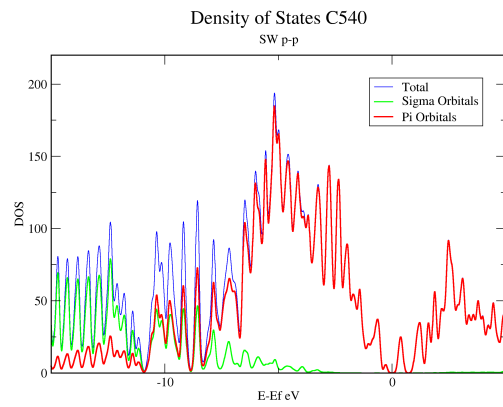
3.33. C₅₄₀ SW h-h



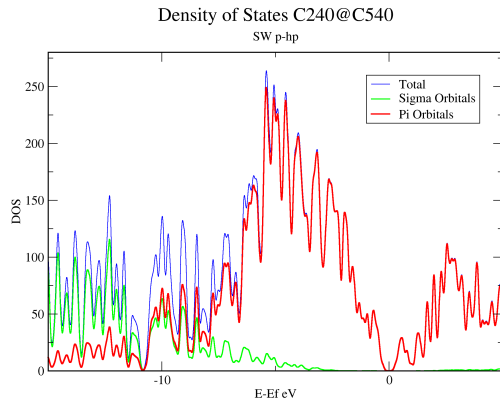
3.34. C₅₄₀ SW hp-h



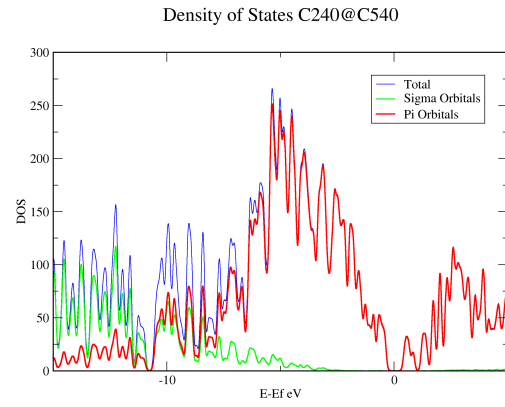
3.35. C₅₄₀ SW p-hp



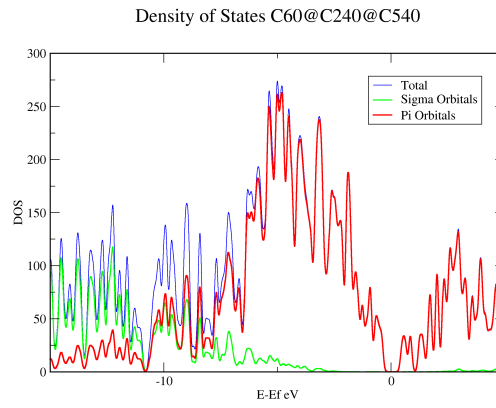
3.36. C₅₄₀ SW p-p



3.37. C₂₄₀@C₅₄₀ SW p-hp



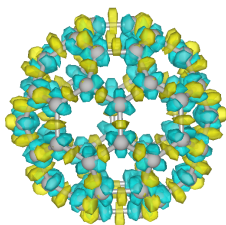
3.38. C₂₄₀@C₅₄₀



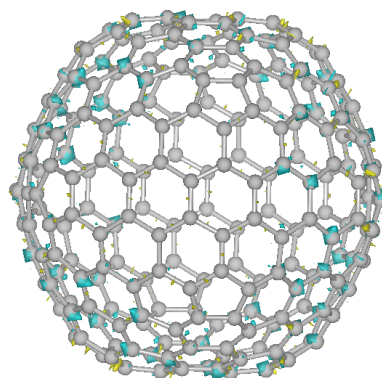
3.39. C₆₀@C₂₄₀@C₅₄₀

Figure 3: Density of States.

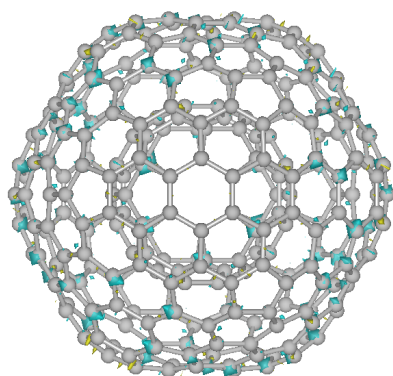
4 Total Charge Difference



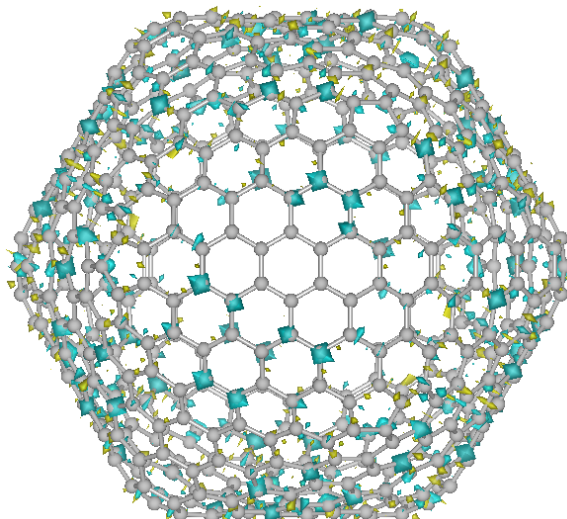
4.1. C_{60}



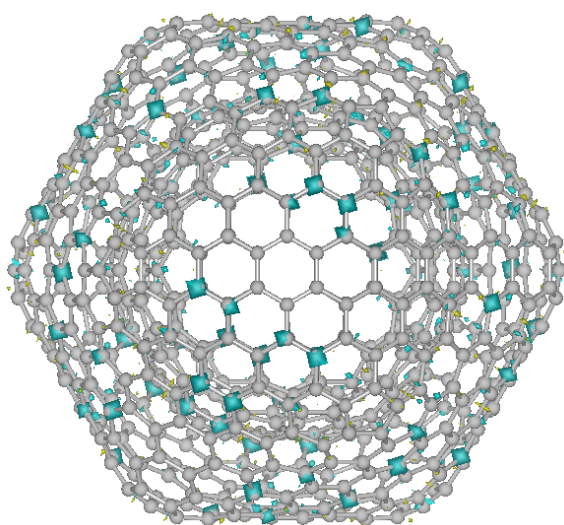
4.2. C_{240}



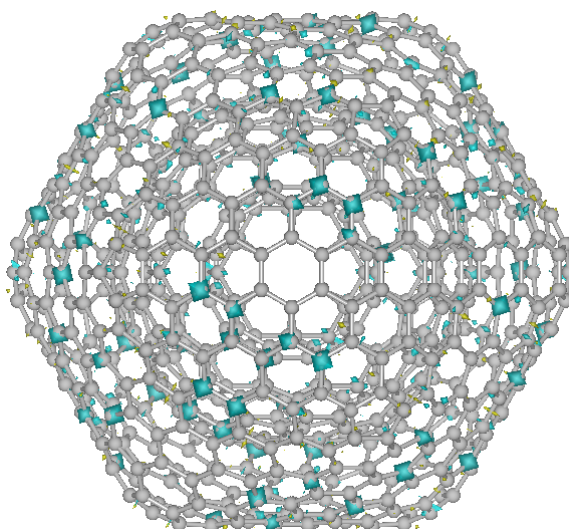
4.3. $C_{60}@C_{240}$



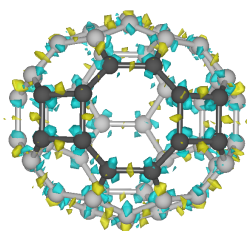
4.4. C_{540}



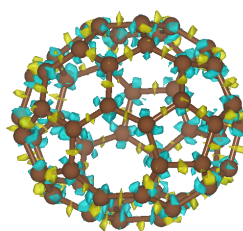
4.5. $C_{240}@C_{540}$



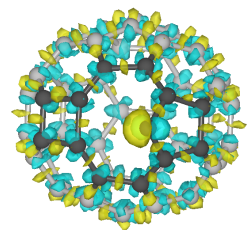
4.6. $C_{60}@C_{240}@C_{540}$



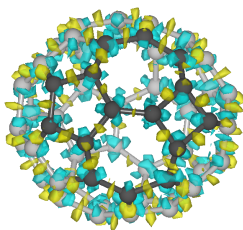
4.7. C₆₀ DV p-hp



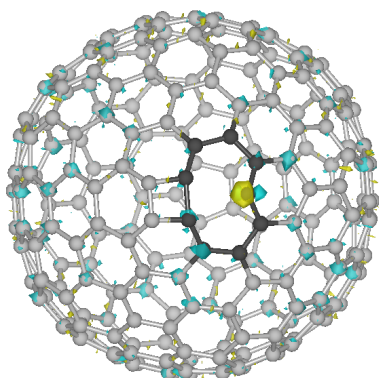
4.8. C₆₀ DV p-p



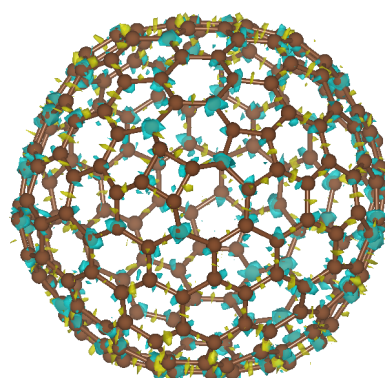
4.9. C₆₀ SV hp



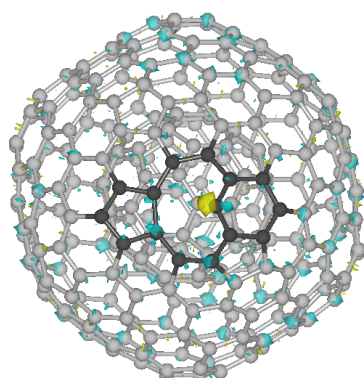
4.10. C₆₀ SW p-p



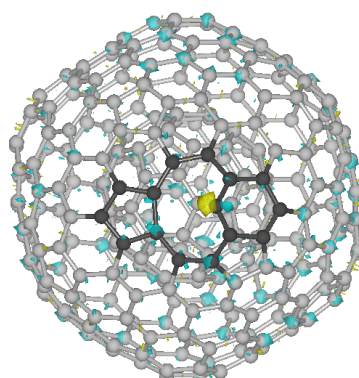
4.11. C₂₄₀ SV p



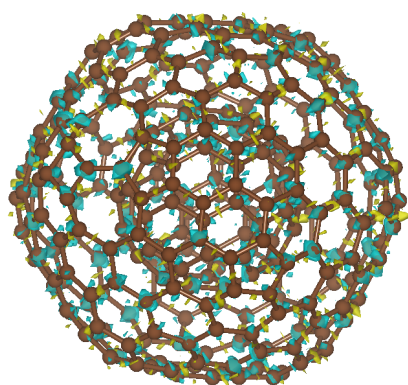
4.12. C₂₄₀ SW p-p



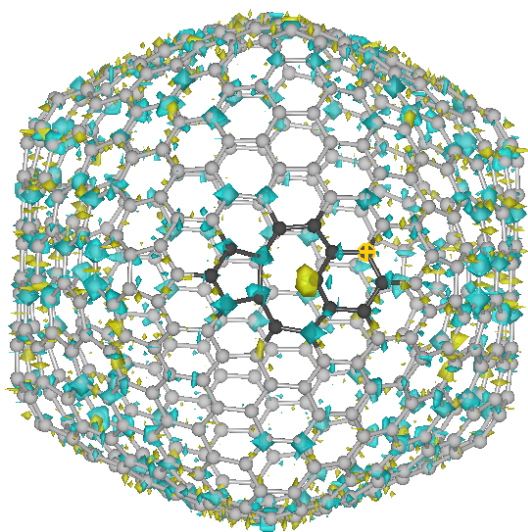
4.13. C₆₀@C₂₄₀ SV h



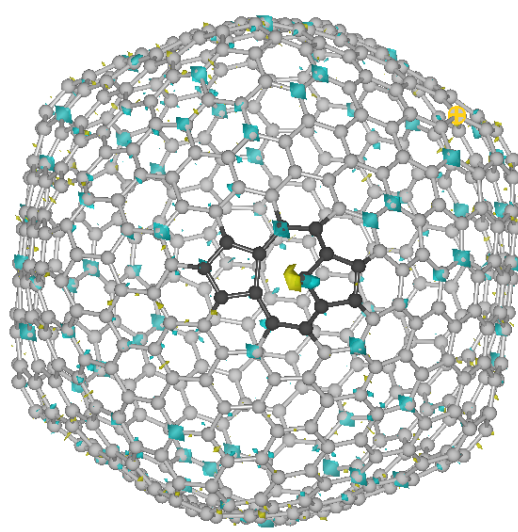
4.14. C₆₀@C₂₄₀ DV h-h



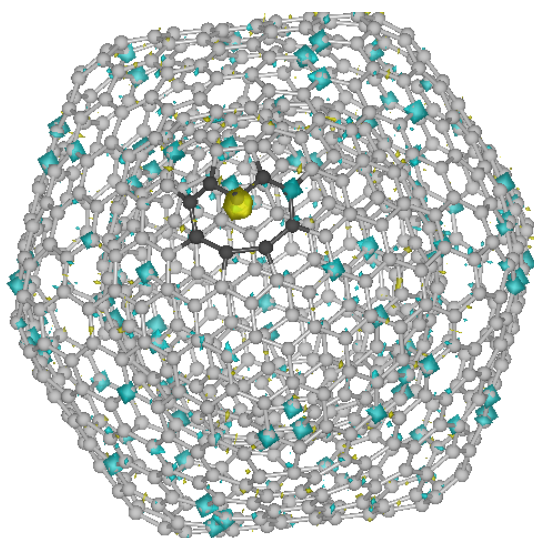
4.15. $C_{60}@C_{240}$ SW p-p



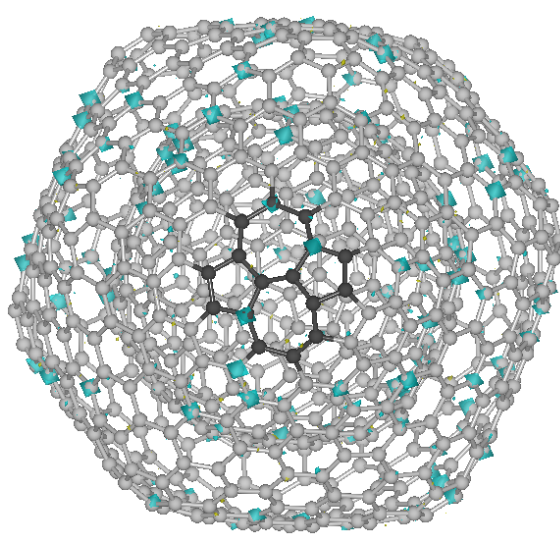
4.16. C_{540} SV h



4.17. C_{540} SV hp



4.18. $C_{240}@C_{540}$ SV h



4.19. $C_{240}@C_{540}$ SW hp-h

Figure 4: Total charge difference.