Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Modeling laser induced molecule excitation using real-time time-dependent density functional theory: Application to 5- and 6-benzyluracil

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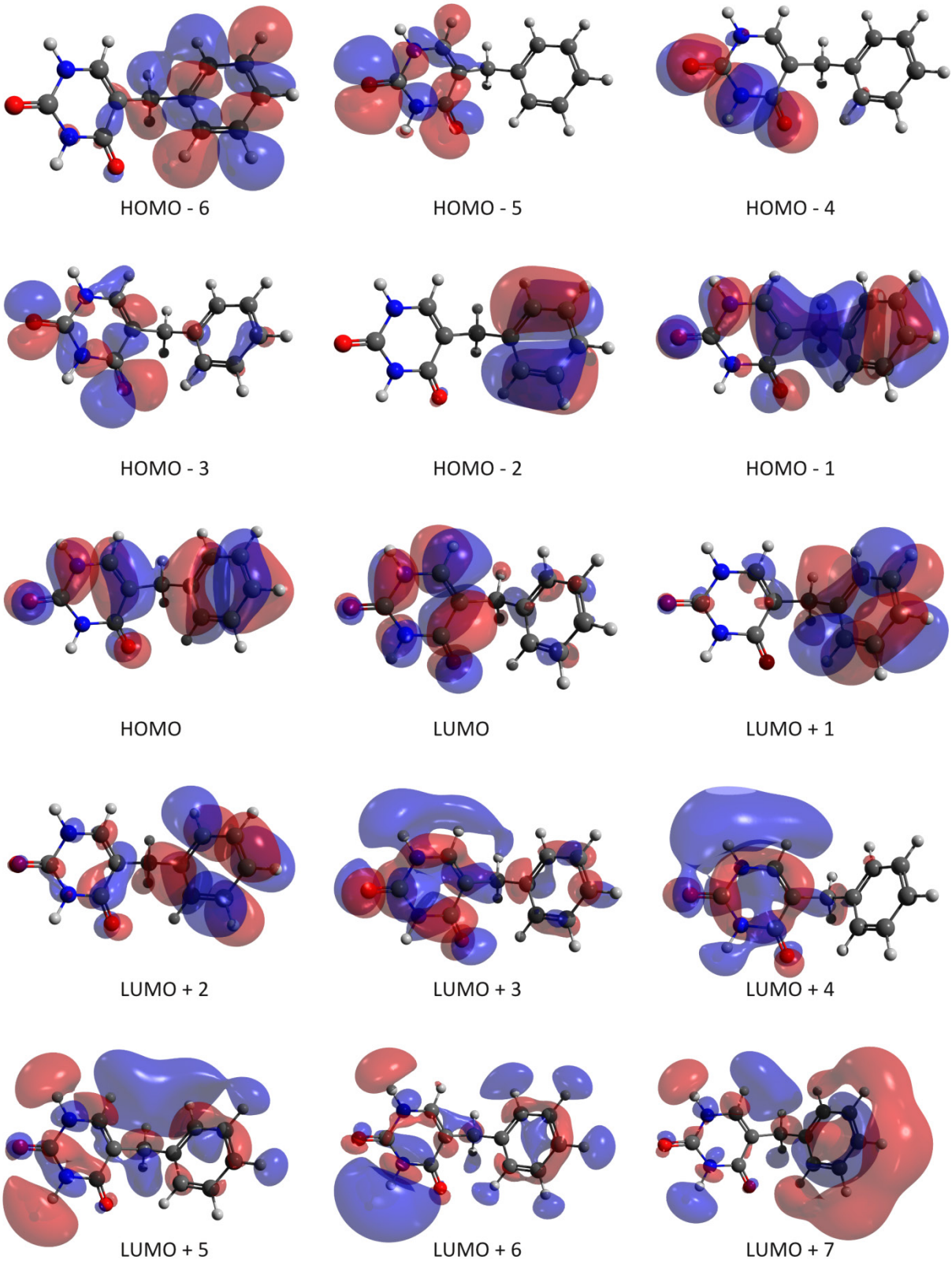


Figure S1. The orbital shapes of the last seven occupied and first eight unoccupied orbitals of the 5BU system.

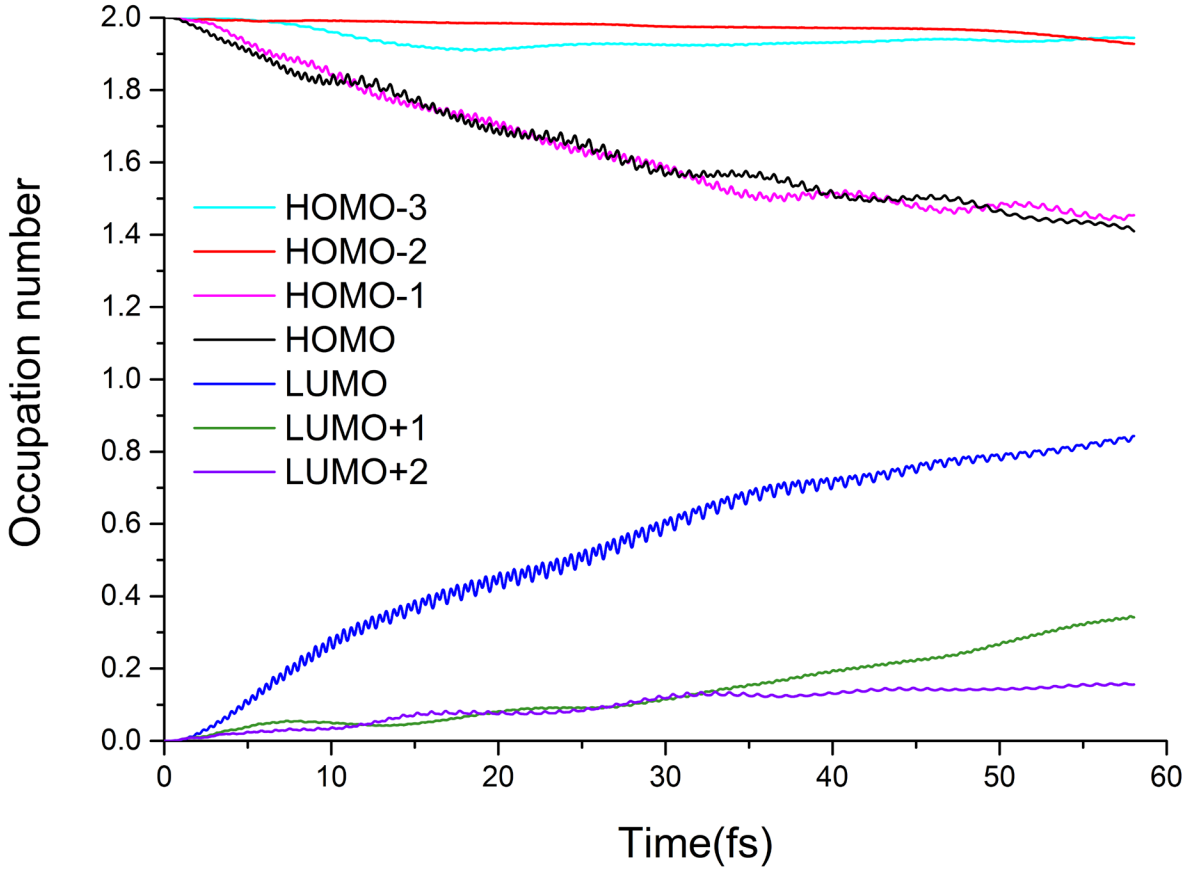


Figure S2. From HOMO-3 to HOMO occupied and from LUMO to LUMO+2 virtual orbital's population induced by a laser field applied in the *Z* directions with 60 fs pulse duration in the case of 5BU system.

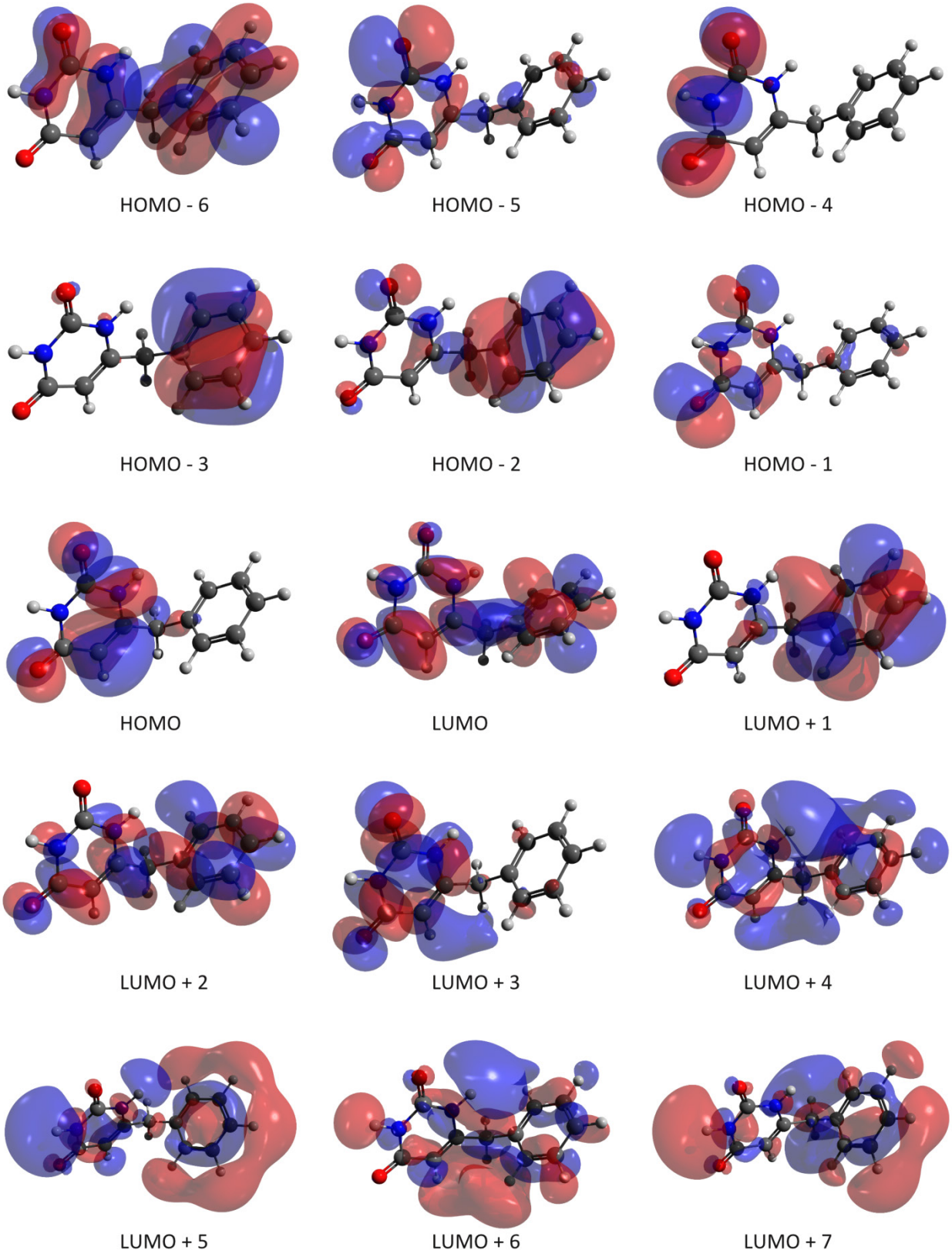


Figure S3. The orbital shapes of the last seven occupied and first eight unoccupied orbitals of the 6BU system.

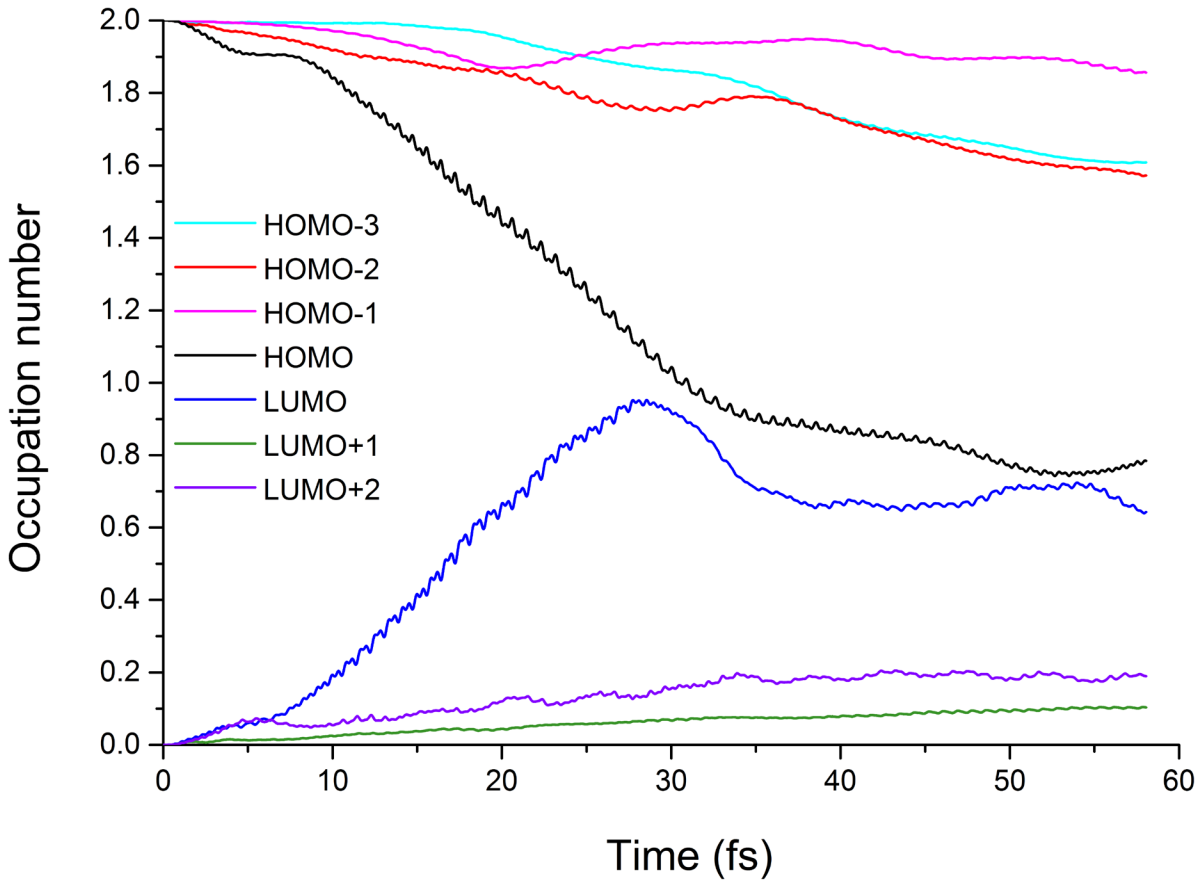
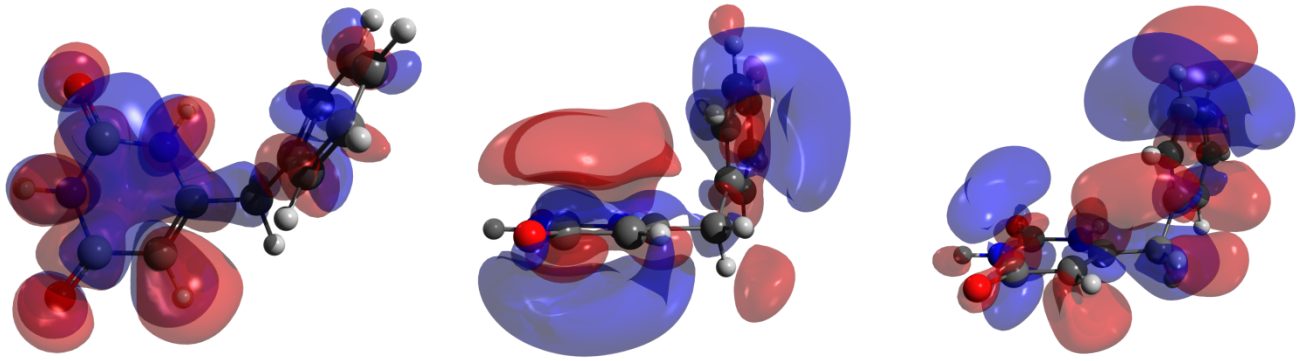


Figure S4. From HOMO-3 to HOMO occupied and from LUMO to LUMO+2 virtual orbital's population induced by a laser field applied in the *Z* directions with 60 fs pulse duration in the case of 6BU system.



LUMO+17 LUMO+21 LUMO+23

Figure S5. The orbital shapes of the 18th, 22nd and 24th unoccupied orbitals of the 6BU system.

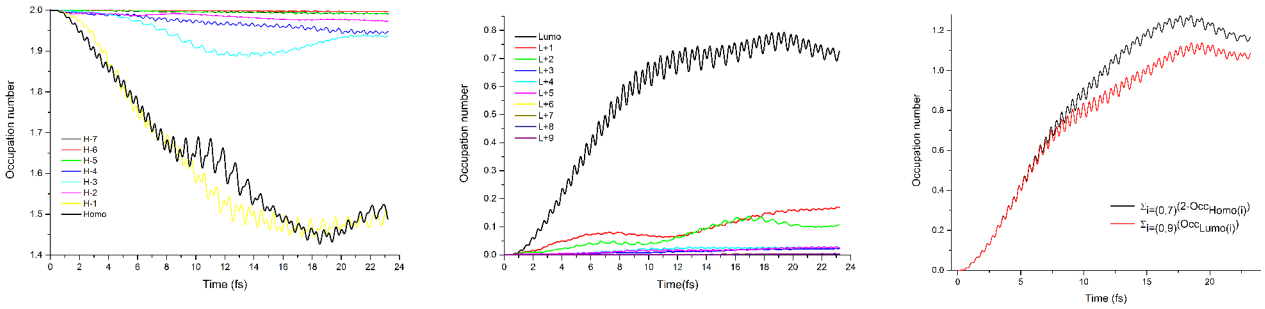


Figure S6. The HOMO, LUMO as well as the total occupied orbital depopulation and the total virtual orbital occupation of 5BU for a laser field in *YZ* direction.

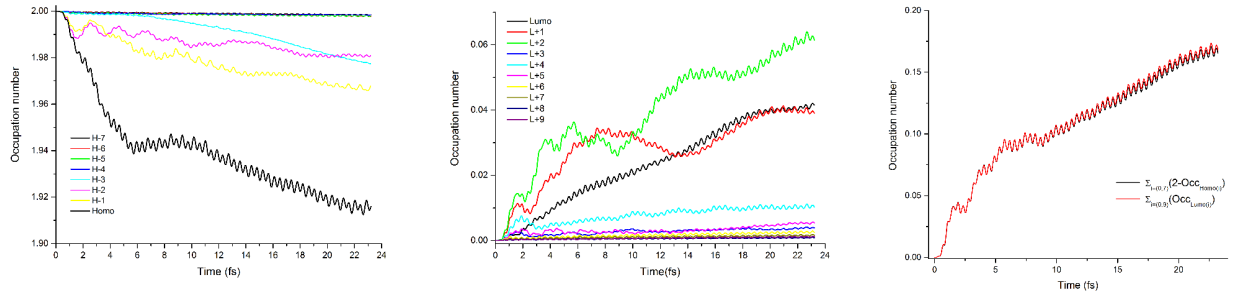


Figure S7. The HOMO, LUMO as well as the total occupied orbital depopulation and the total virtual orbital occupation of 5BU for a laser field in *-YZ* direction.

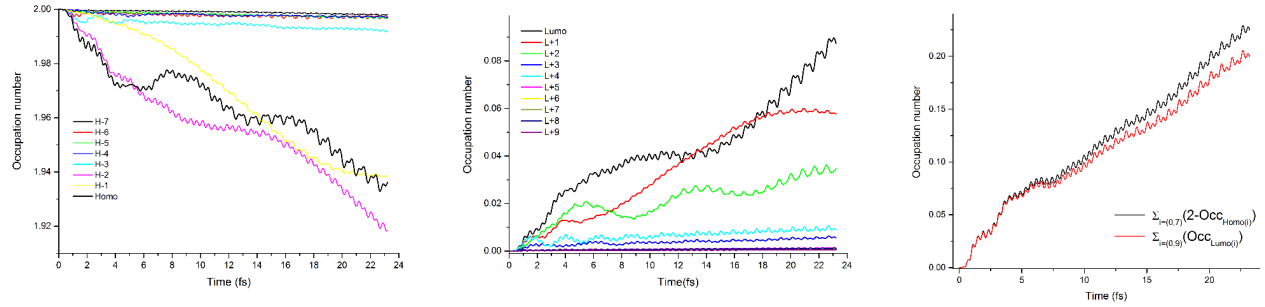


Figure S8. The HOMO, LUMO as well as the total occupied orbital depopulation and the total virtual orbital occupation of 6BU for a laser field in *YZ* direction.

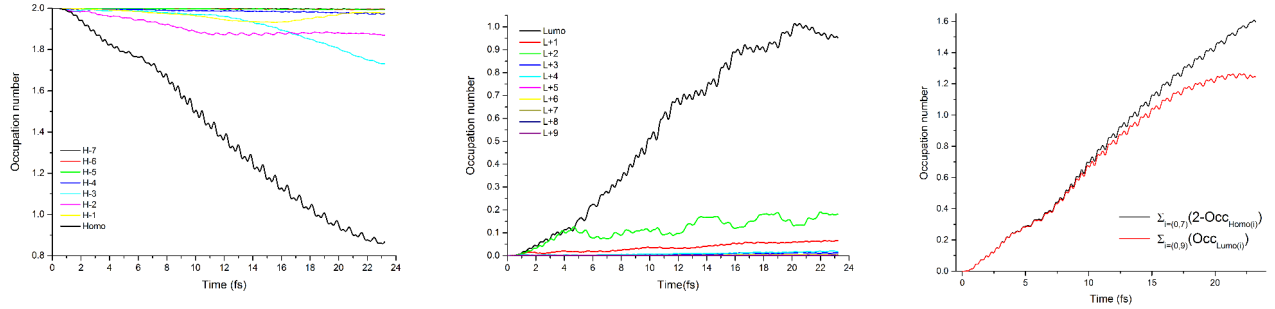


Figure S9. The HOMO, LUMO as well as the total occupied orbital depopulation and the total virtual orbital occupation of 6BU for a laser field in *-YZ* direction.

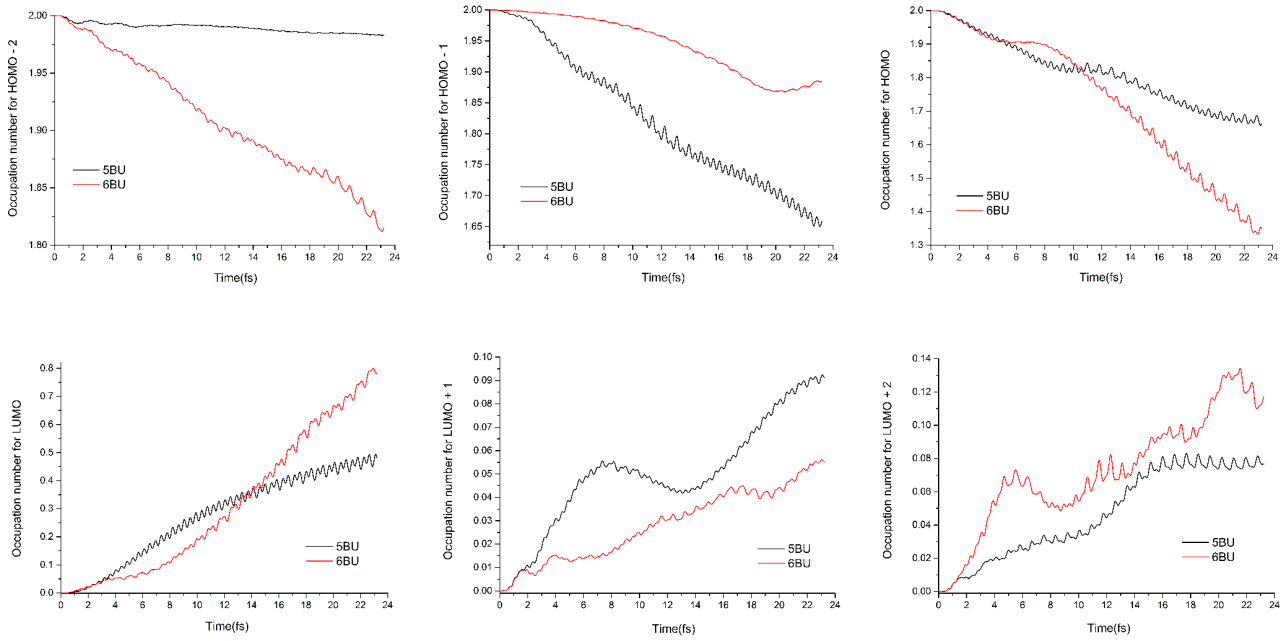


Figure S10.The HOMO - 2, HOMO - 1, HOMO, LUMO, LUMO + 1 and LUMO + 2 orbital population for 5BU and 6BU molecular systems.

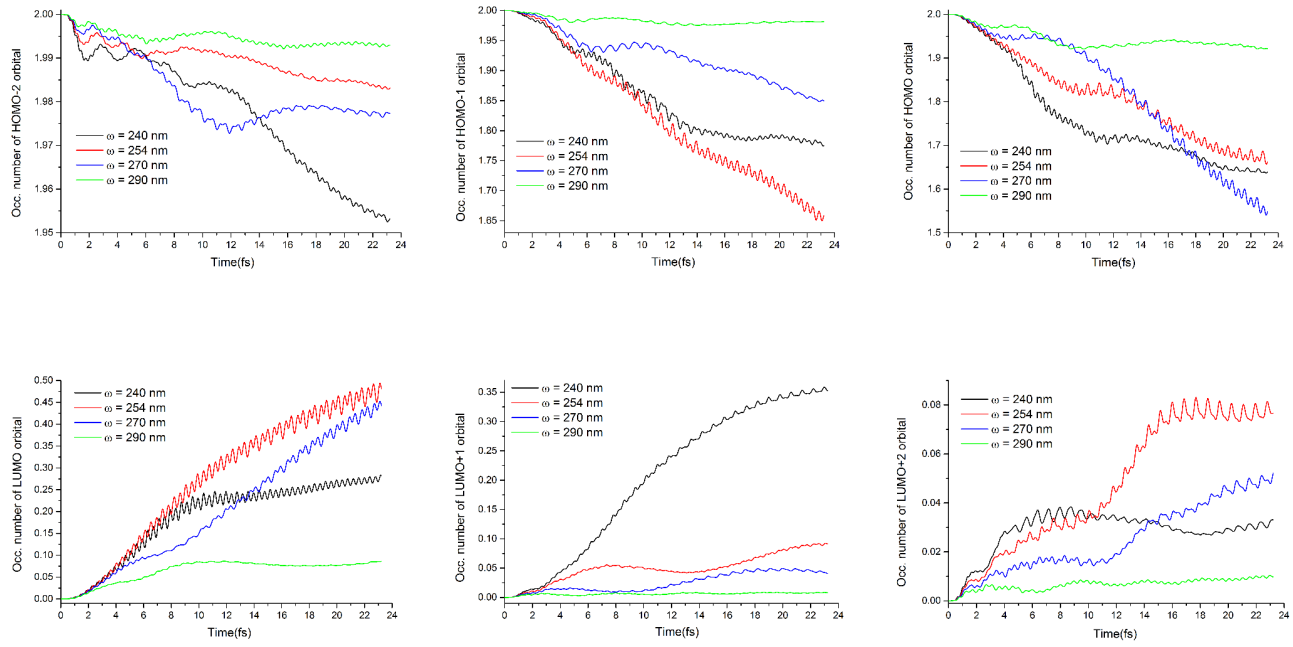


Figure S11. The HOMO - 2, HOMO - 1, HOMO, LUMO, LUMO + 1 and LUMO + 2 orbital populations for 5BU molecular system using four different (240 nm, 254 nm, 270 nm and 290 nm) laser frequencies in the direction of *Z* axis.

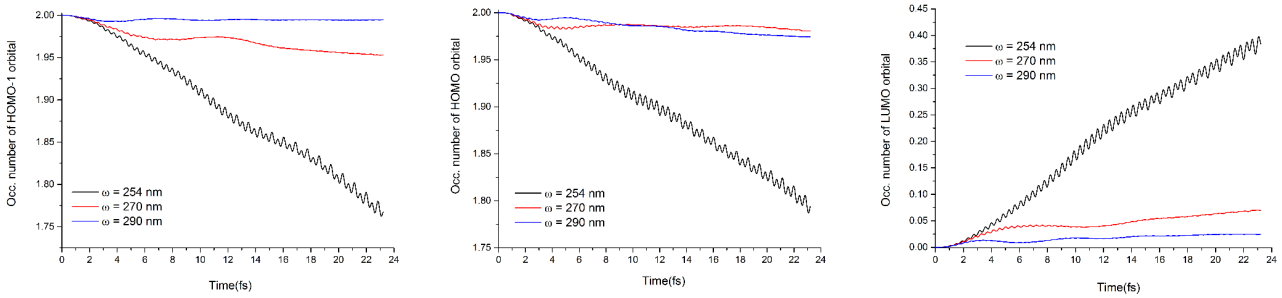


Figure S12. The HOMO - 1, HOMO, LUMO orbital populations for 5BU molecular system using four different (254 nm, 270 nm and 290 nm) laser frequencies in the direction of *Y* axis.

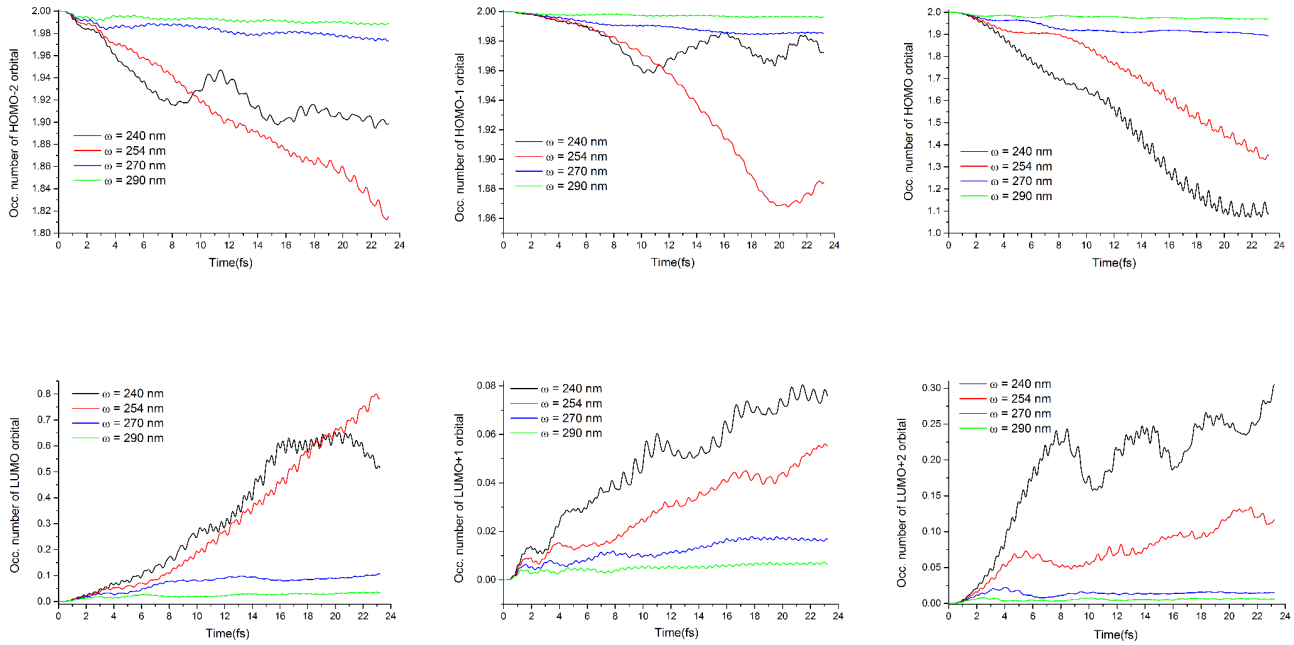


Figure S13. The HOMO - 2, HOMO - 1, HOMO, LUMO, LUMO + 1 and LUMO + 2 orbital populations for 6BU molecular system using four different (240 nm, 254 nm, 270 nm and 290 nm) laser frequencies in the direction of *Z* axis.

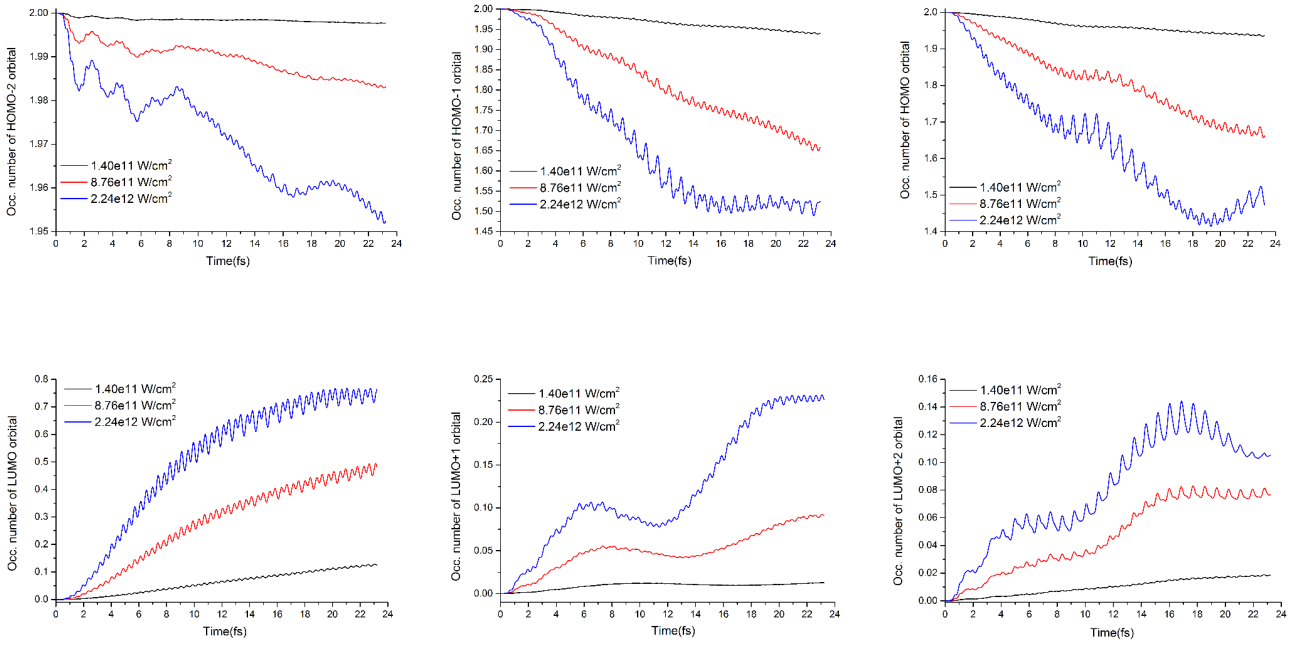


Figure S14. The HOMO - 2, HOMO - 1, HOMO, LUMO, LUMO + 1 and LUMO + 2 orbital populations for 5BU molecular system using three different (1.40e11 W/cm^2, 8.76e11 W/cm^2 and 2.24e12 W/cm^2) laser intensities in the direction of *Z* axis.

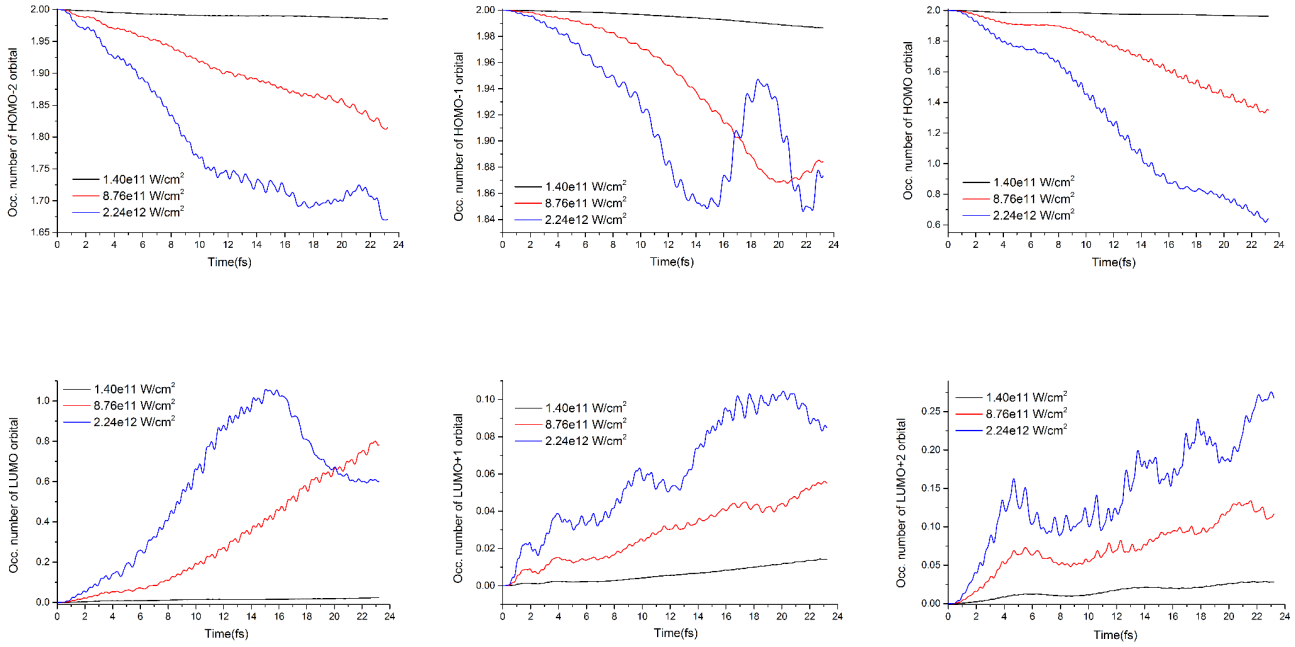


Figure S15. The HOMO - 2, HOMO - 1, HOMO, LUMO, LUMO + 1 and LUMO + 2 orbital populations for 6BU molecular system using three different (1.40e11 W/cm^2, 8.76e11 W/cm^2 and 2.24e12 W/cm^2) laser intensities in the direction of *Z* axis.