

Supporting Information

Ab Initio Investigation of the Ground States of F₂P(S)N, F₂PNS, and F₂PSN

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Figure S1. The active orbitals of CAS(12,10) for $\text{F}_2\text{P}(\text{S})\text{N}$.

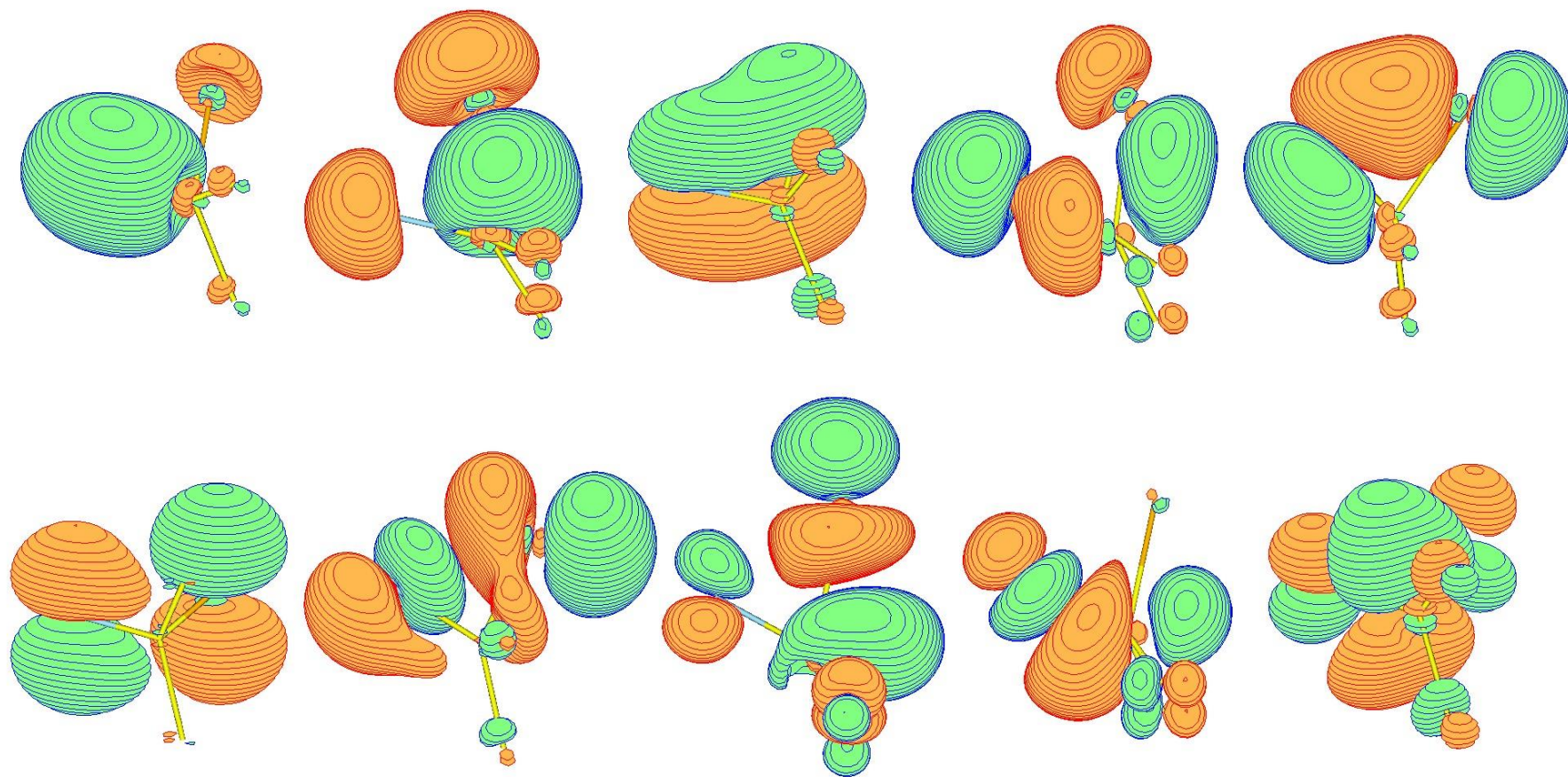


Figure S2. The active orbitals of CAS(12,10) for F₂PNS.

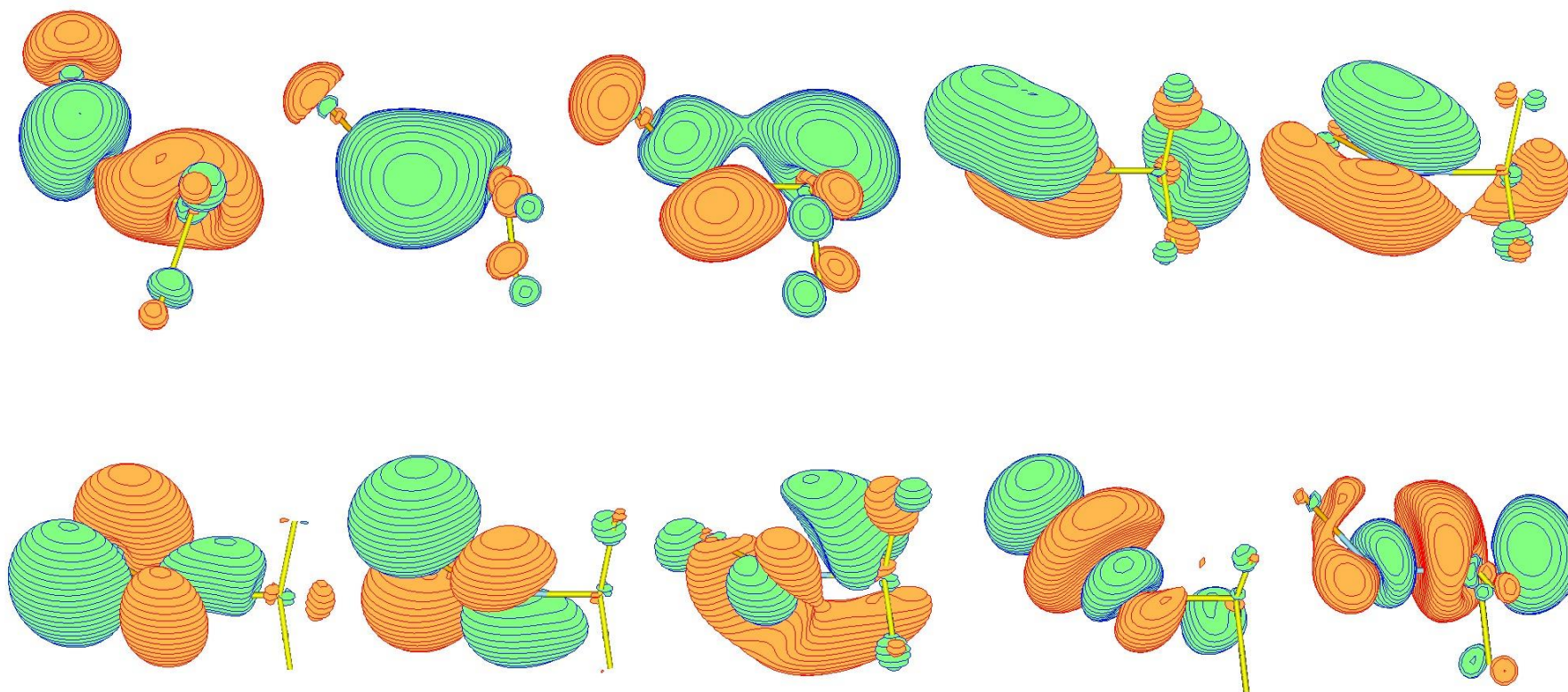


Figure S3. The active orbitals of CAS(10,9) for F₂PSN.

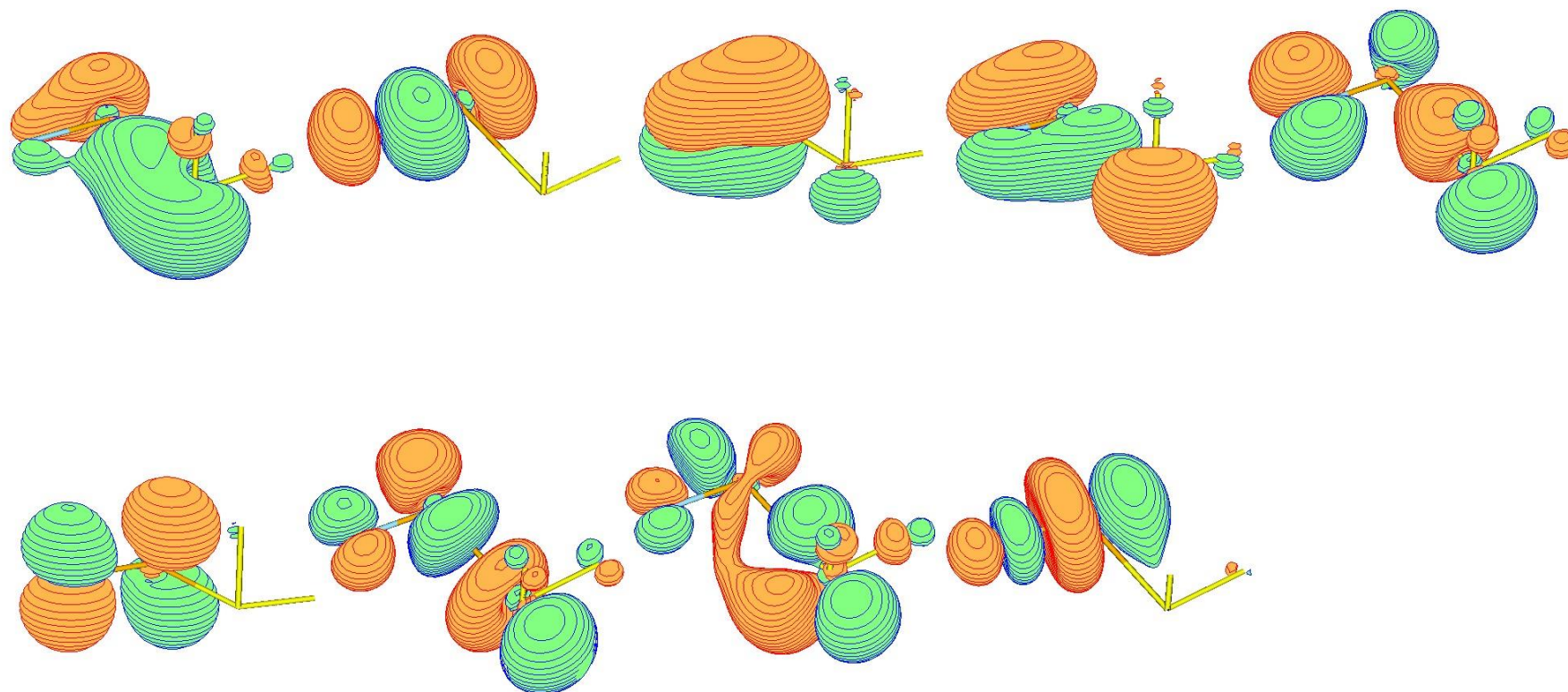


Table S1. The harmonic and anharmonic vibrational frequencies (in cm⁻¹) of the singlet state of F₂PSN calculated by DFT method

Vibration Mode	B3LYP		B3PW91		APFD		PBE0	
	harmonic	anharmonic	harmonic	anharmonic	harmonic	anharmonic	harmonic	anharmonic
PF ₂ rocking	14.8	182.5	10.2	54.0 <i>i</i>	10.4	84.2 <i>i</i>	2.7	1179.7
PF ₂ wagging	137.0	143.4	138.0	109.0	109.6	80.5	141.6	16.8
PF ₂ twisting	190.0	189.6	197.9	197.3	218.0	200.4	208.9	213.2
PS stretch.	140.3	150.5	143.4	153.5	192.7	169.3	150.1	163.9
PF ₂ scissoring	346.6	344.8	351.5	344.1	358.5	351.1	358.0	340.7
PSN bend.	467.5	462.7	480.1	468.2	470.6	415.4	496.4	470.0
PF ₂ asym. stretch.	796.7	787.6	812.0	801.5	824.9	813.1	825.6	818.1
PF ₂ sym. stretch.	808.3	798.3	821.9	811.0	832.0	822.2	835.2	827.1
SN stretch.	1184.8	1172.7	1201.1	1177.8	1198.9	1179.5	1203.6	1187.8

Figure S4. The active orbitals of CAS(14,11) for $\text{F}_2\text{P}(\text{S})\text{N}$ in the T_v s calculation.

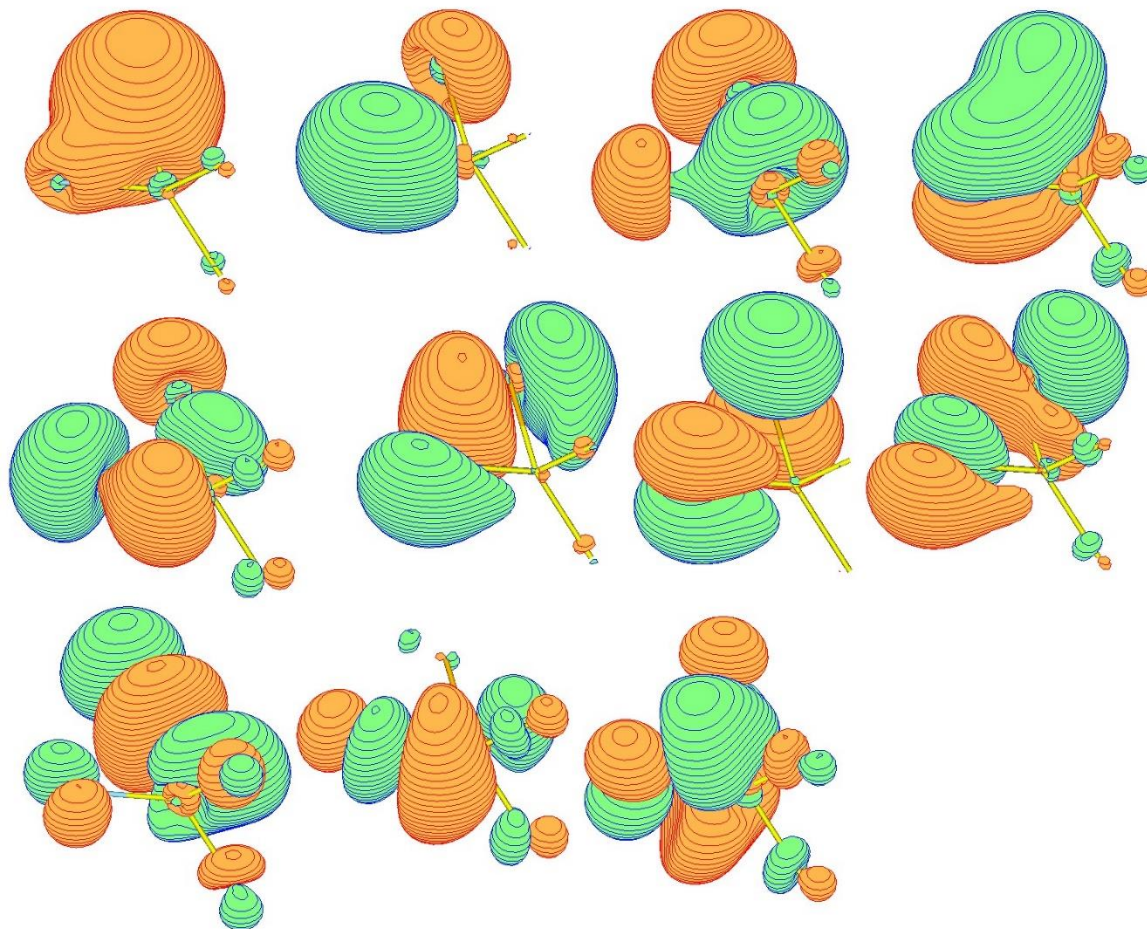


Figure S5. The active orbitals of CAS(14,11) for F₂PNS in the T_vs calculation.

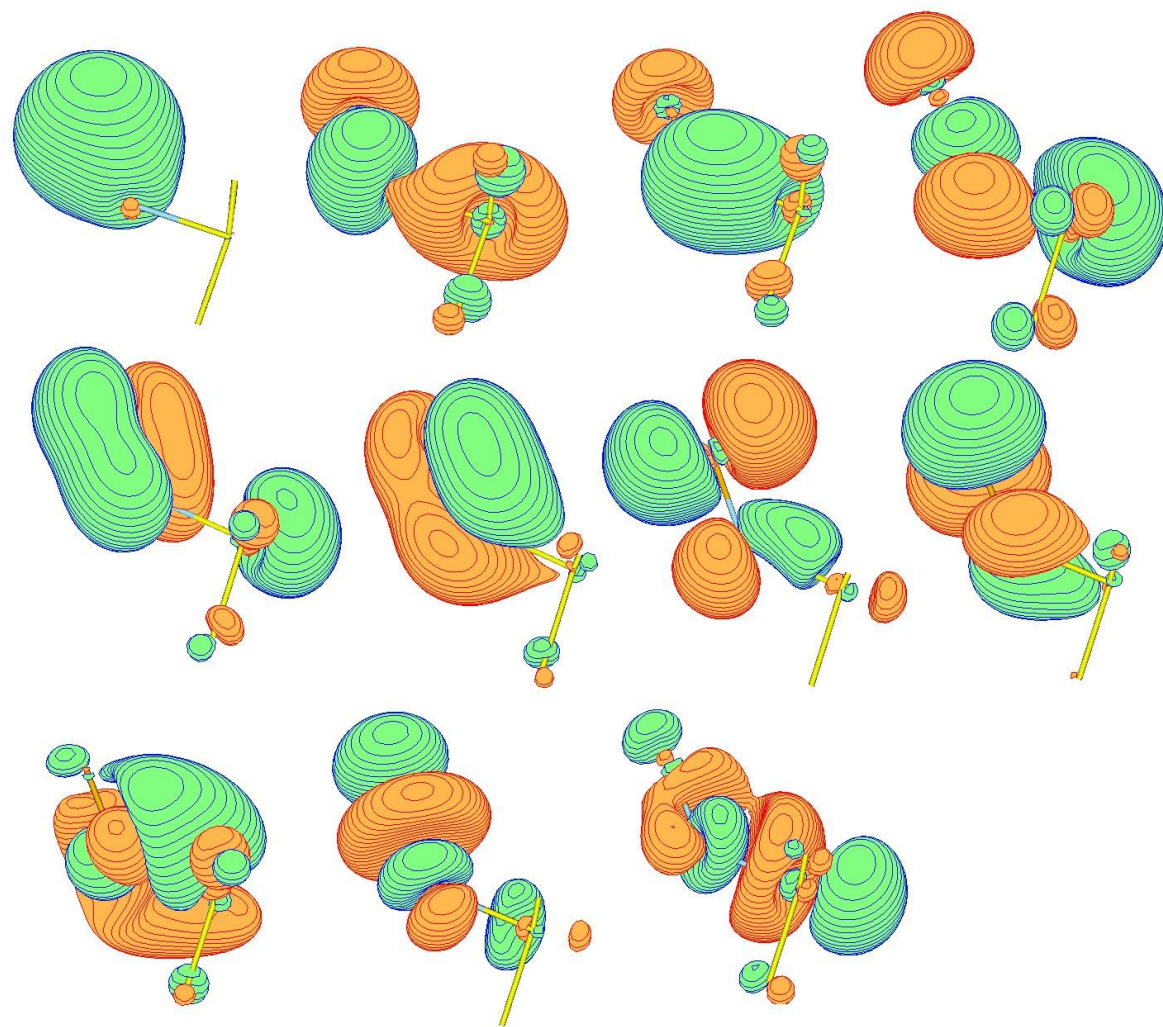


Figure S6. The active orbitals of CAS(14,11) for F₂PSN in the T_vs calculation.

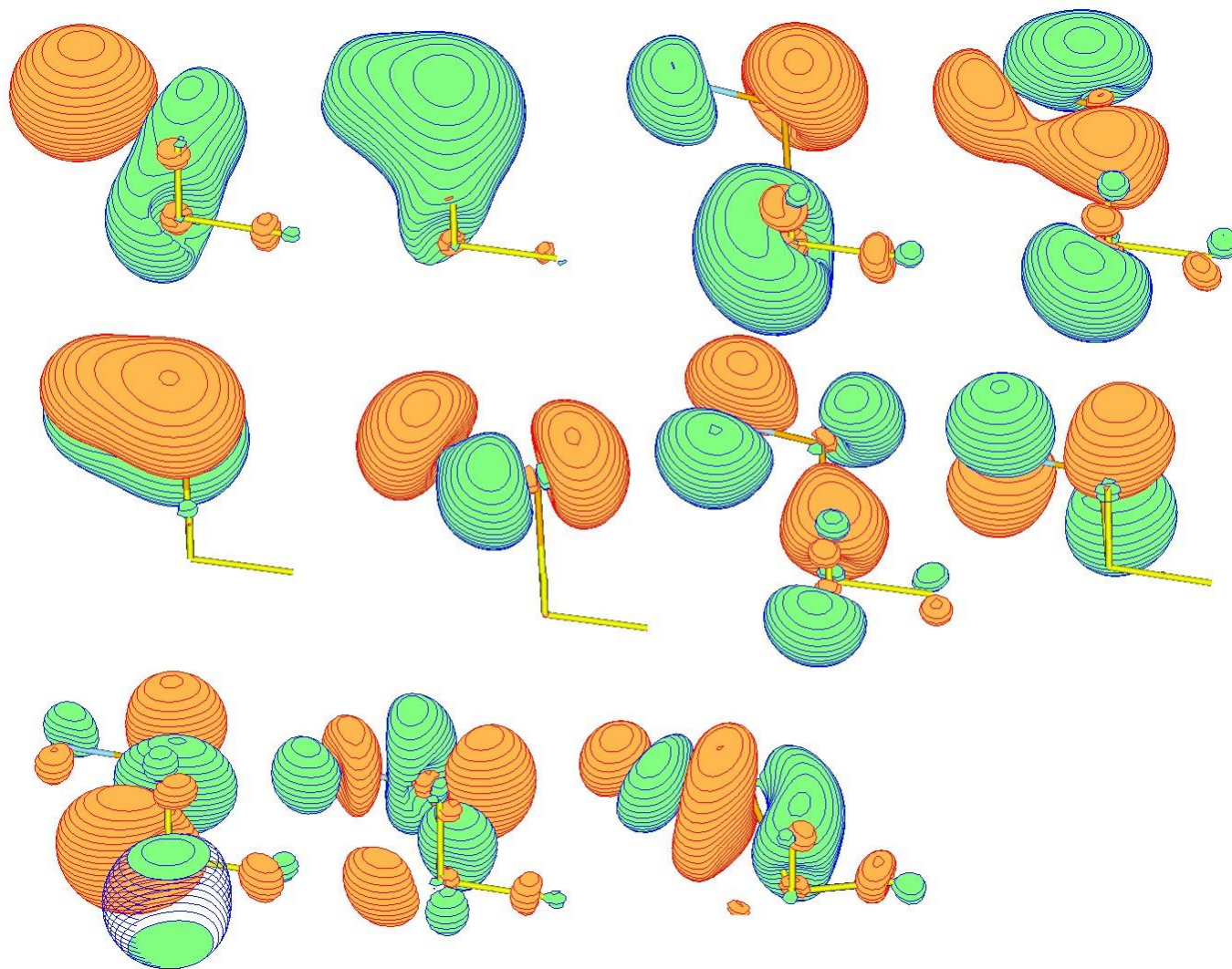


Figure S7. The calculated UV-vis spectrum of $F_2P(S)N$, F_2PNS , and F_2PSN based on the MS-CASPT2 calculations. The absorption peaks were represented by Gaussian functions. The standard deviation of 0.4 eV was used for Gaussian function.

