



ELECTRONIC, LIGHT HARVESTING EFFICIENCY AND DYNAMIC OPTICAL PROPERTIES OF NITROBENZYLIDENE SCHIFF BASES USING DENSITY FUNCTIONAL THEORY

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INTRODUCTION

As sustainability becomes a more pressing concern, organic compounds such as Schiff bases support the objectives of promoting green technologies and reducing environmental effects.

Why Schiff bases?

- ❖ Schiff have good electrical and optical properties.
- ❖ Schiff bases are inexpensive
- ❖ Easily tunable at the molecular level
- ❖ They have minimal toxicity
- ❖ Easy to synthesize

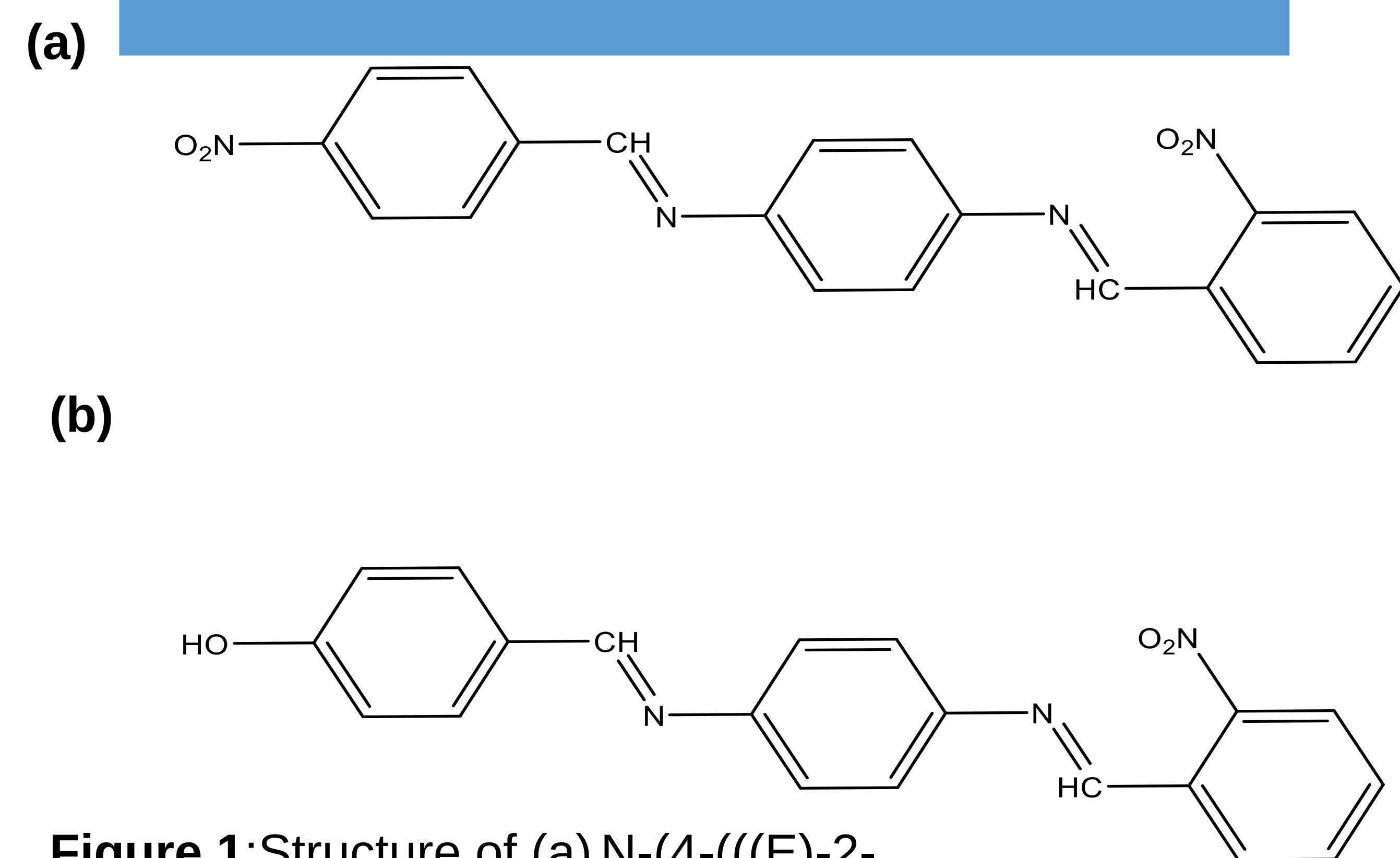
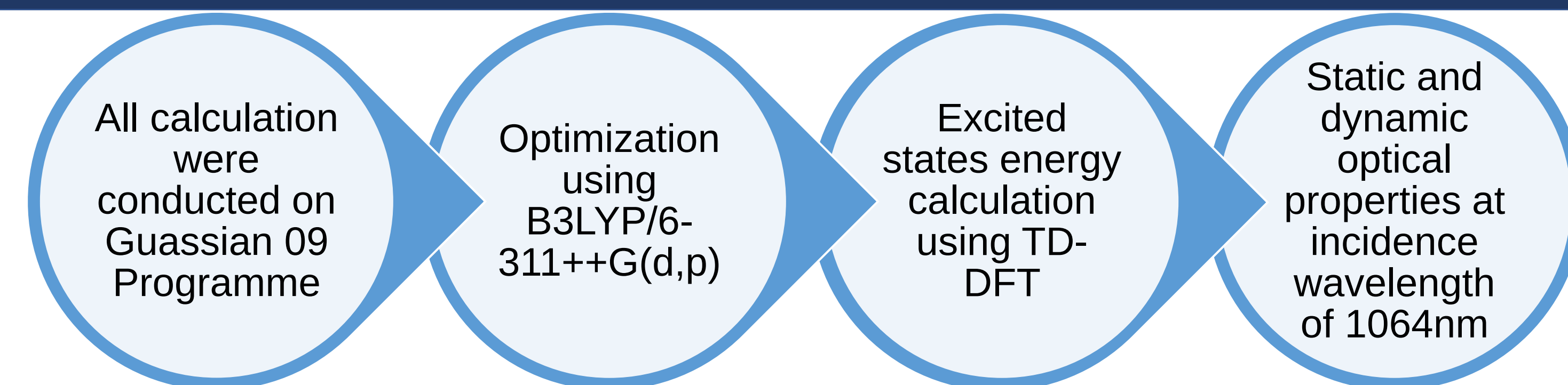


Figure 1: Structure of (a) N-(4-(((E)-2-nitrobenzylidene)amino)phenyl)-1-(4-nitrophenyl)methanimine (NNM) and (b) 4-(((4-((2-nitrobenzylidene)amino)phenyl)imino)methyl)phenol (NMP)

AIM

To study the electronic, light harvesting efficiency (LHE) and dynamic optical properties of two nitrobenzylidene Schiff bases, N-(4(((E)-2nitrobenzylidene) amino) phenyl)-1-(4-nitrophenyl)methanimine(NNM), and 4(((4((2nitrobenzylidene)amino)phenyl)imino)methyl)phenol (NMP) using Density functional theory (DFT).

METHODS



RESULTS

Table 1: Frequency-dependent ($\beta \times 10^{-51} \text{ C}^3\text{m}^3\text{J}^{-2}$; $\gamma \times 10^{-61} \text{ C}^4\text{m}^4\text{J}^{-3}$) NLO properties of NNM and NMP at 1064 nm ($\hbar\omega = 0.042822\text{au}$)

Compound	$\beta_{ }$	β_{tot}	$B(-2w;w,w)$	$\beta(-w;w,0)$	$\beta(0;0,0)$	$\gamma_{ }(-2w;w,w,0)$	$\gamma_{ }(-w;w,0,0)$	$\gamma_{ }(0;0,0,0)$
NNM	2428	559	1460	335	211	10247	1796	1100
NMP	1237	381	744	277	200	3469	1009	684

Urea: $\beta(0;0,0) = 1.73$; $\beta(-w;w,0) = 1.86$; $\beta(-2w;w,w) = 2.04$; $\gamma_{||}(-2w;w,w,0) = 6.25$; $\gamma_{||}(-w;w,0,0) = 5.47$; $\gamma_{||}(0;0,0,0) = 5.04$ [Units: ($\beta \times 10^{-51} \text{ C}^3\text{m}^3\text{J}^{-2}$; $\gamma \times 10^{-61} \text{ C}^4\text{m}^4\text{J}^{-3}$)]

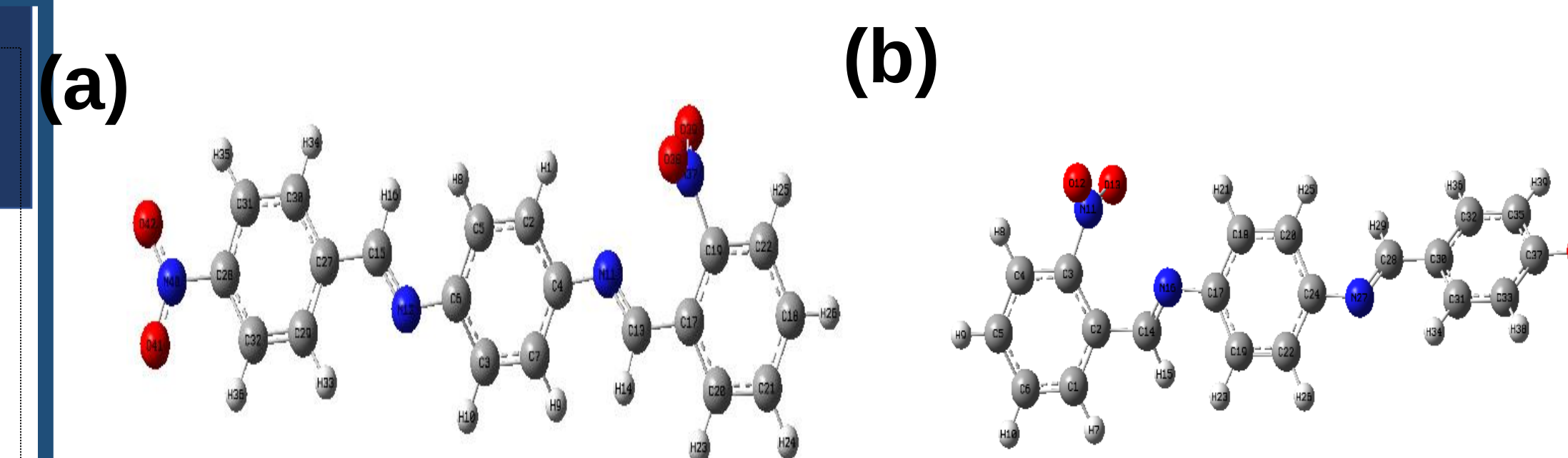


Figure 2: Optimized structures of (a) NNM and (b) NMP

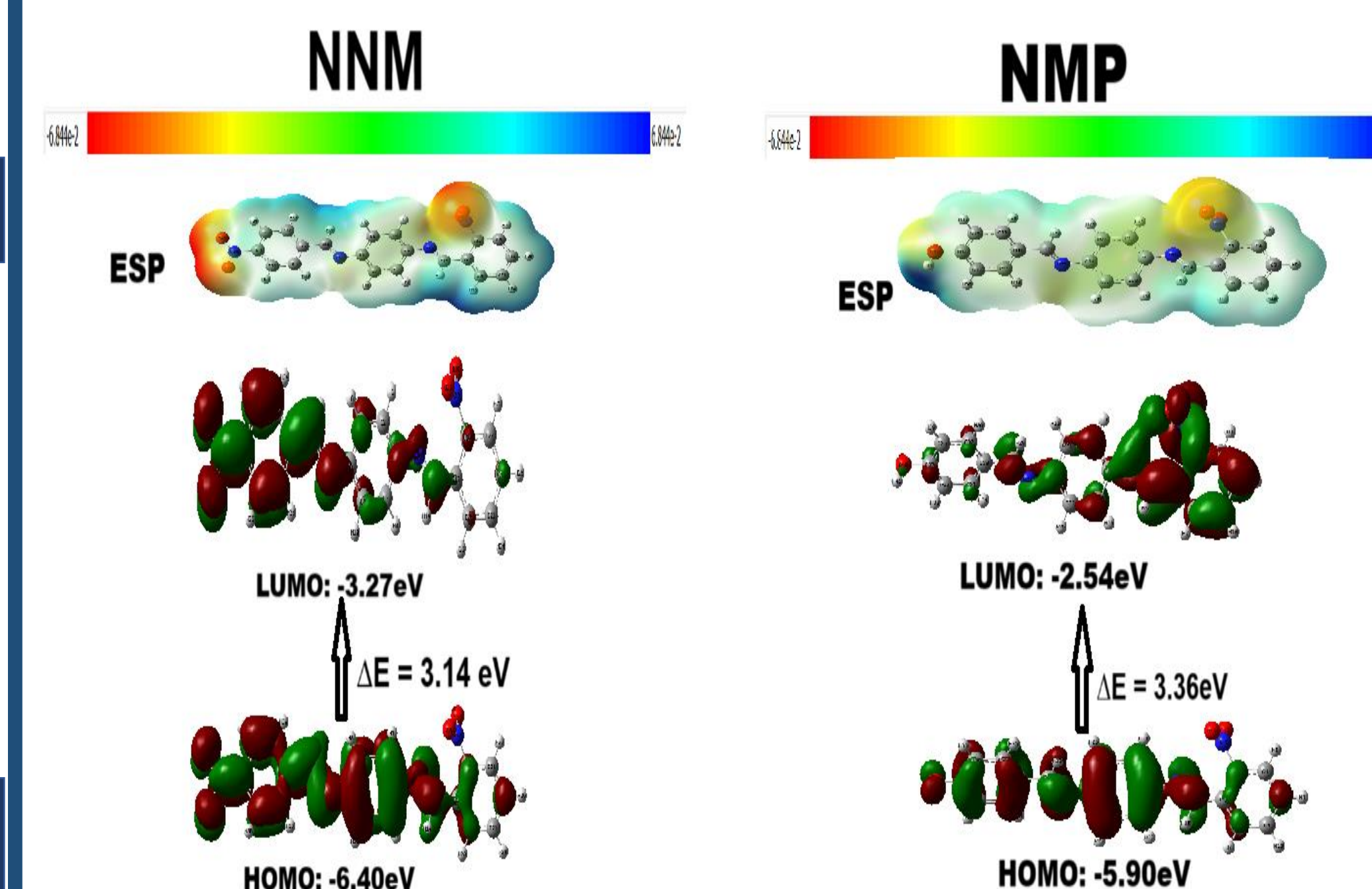


Figure 3: Electrostatic potential map(ESP), HOMO and LUMO of NNM and NMP

Compound	NNM	NMP
LHE in Vacuum (%)	80	74
LHE in Cyclohexane (%)	81	85
LHE in Acetonitrile (%)	83	91

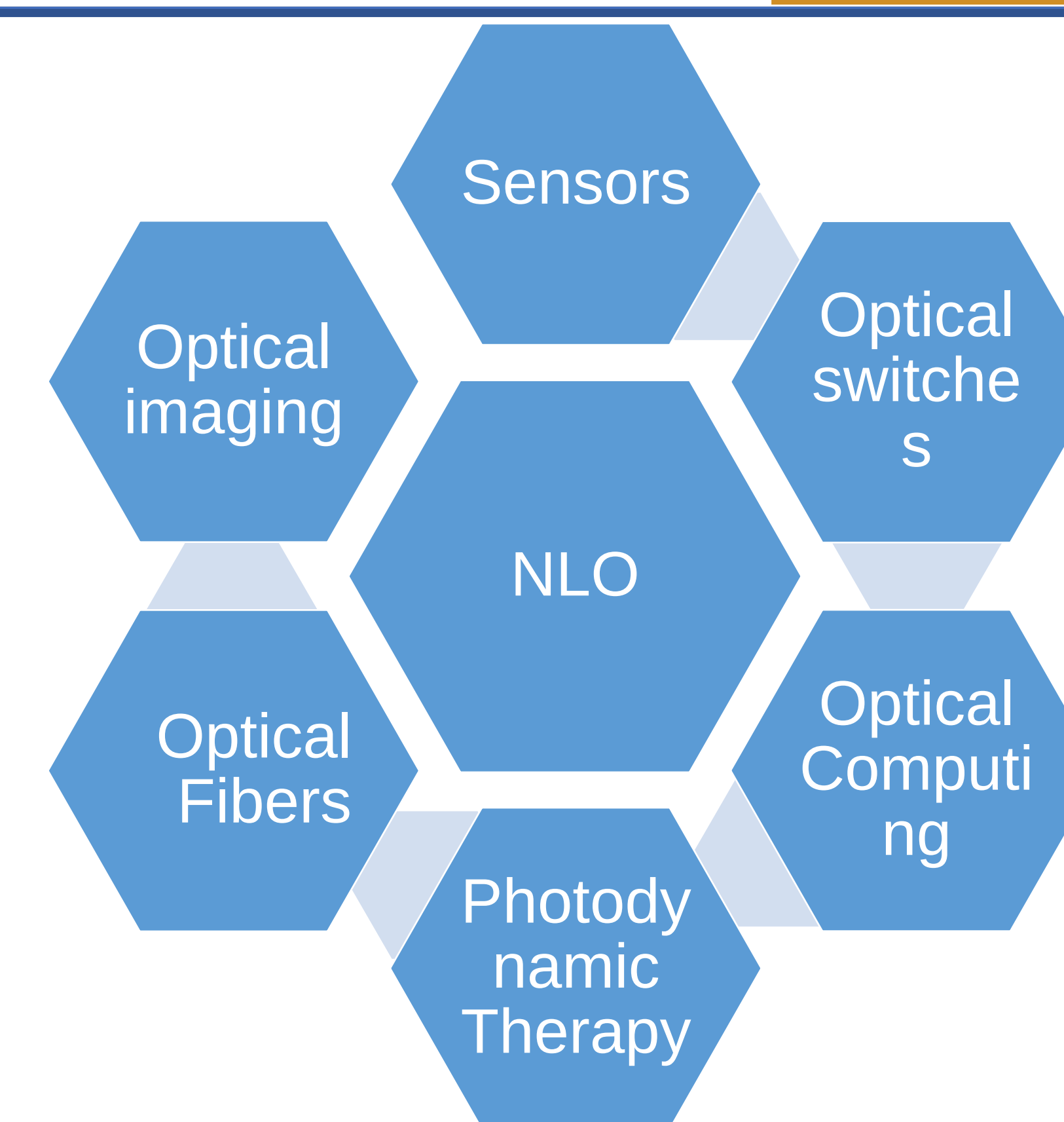


Figure 4: Applications of nonlinear optical materials

CONCLUSION

- ❖ The electronic absorption and light harvesting efficiency (LHE) of the system is solvent-sensitive.
- ❖ NNM and NMP have much higher nonlinear optical properties than urea.
- ❖ The low ΔE , high LHE and large hyperpolarizabilities suggests the potential of the compounds for optoelectronic and nonlinear optical applications.

REFERENCES

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- Oladipupo et al., 2023. Effects of solvent on electronic absorption spectra.. *Scientia Africana*, 22.1:243–254