



Computational Study of Electronic and Nonlinear Optical Properties of (E)-N-(4-(((E)-3-nitrobenzylidene)amino)phenyl)-1-(4-nitrophenyl)methanimine (NAM)



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INTRODUCTION

- ❑ In today's technology-driven world, electricity and heat produce 29% of GHG emissions (IEA, 2023).
- ❑ The demand for smart energy-efficient devices and renewable energy sources (solar energy) continues to rise.
- ❑ While inorganic nonlinear optical materials are mostly used, the high cost and complex production limit their applications.
- ❑ Schiff bases, with their non-toxicity, better semiconduction and electronic properties, high optical nonlinearity, and ease of synthesis, offer a promising organic alternative. (SDG 7 and 12)

Research Question

- ❑ Can NAM be applied in photonic and optoelectronic systems

Aim

- ❑ To Investigate the electronic and Nonlinear Optical (NLO) properties of NAM

COMPUTATIONAL METHOD



Density Functional Theory
Functional: B3LYP
Basis set: 6-311++ G(d,p)
Solvent: vacuum, n-hexane, cyclohexane, tetrachloromethane, dichloromethane, ethanol, methanol, and acetonitrile

Key Parameters

- ❑ HOMO-LUMO energy gap
- ❑ Global reactivity descriptors

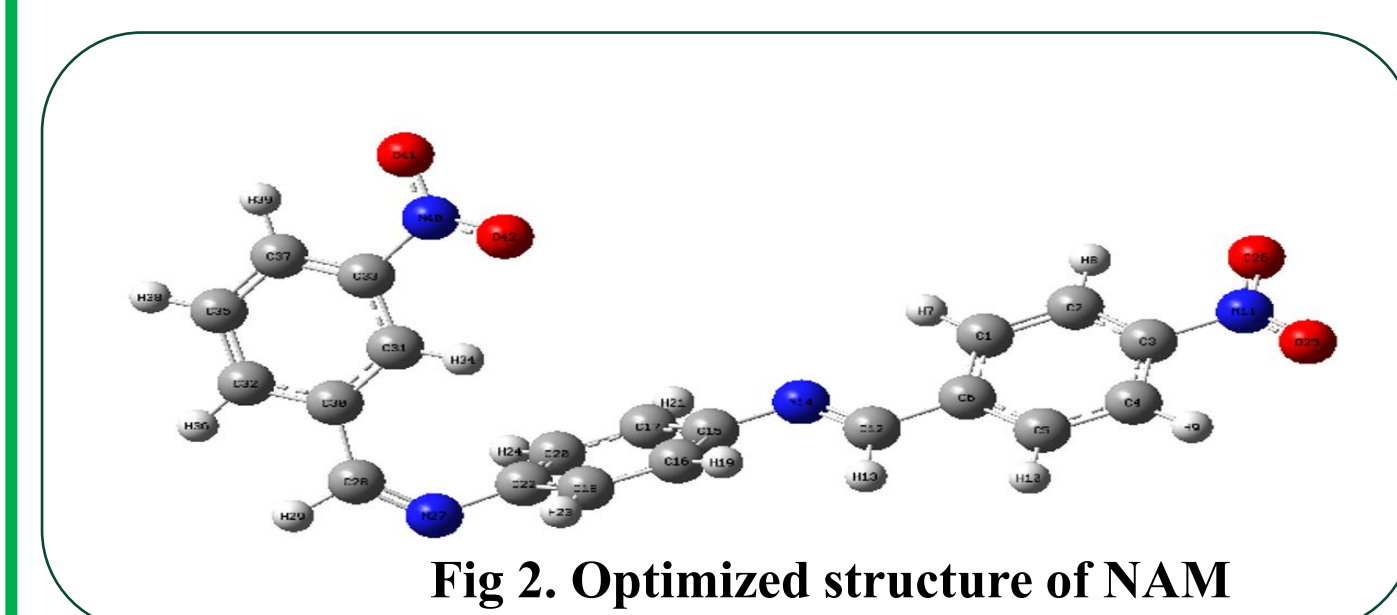
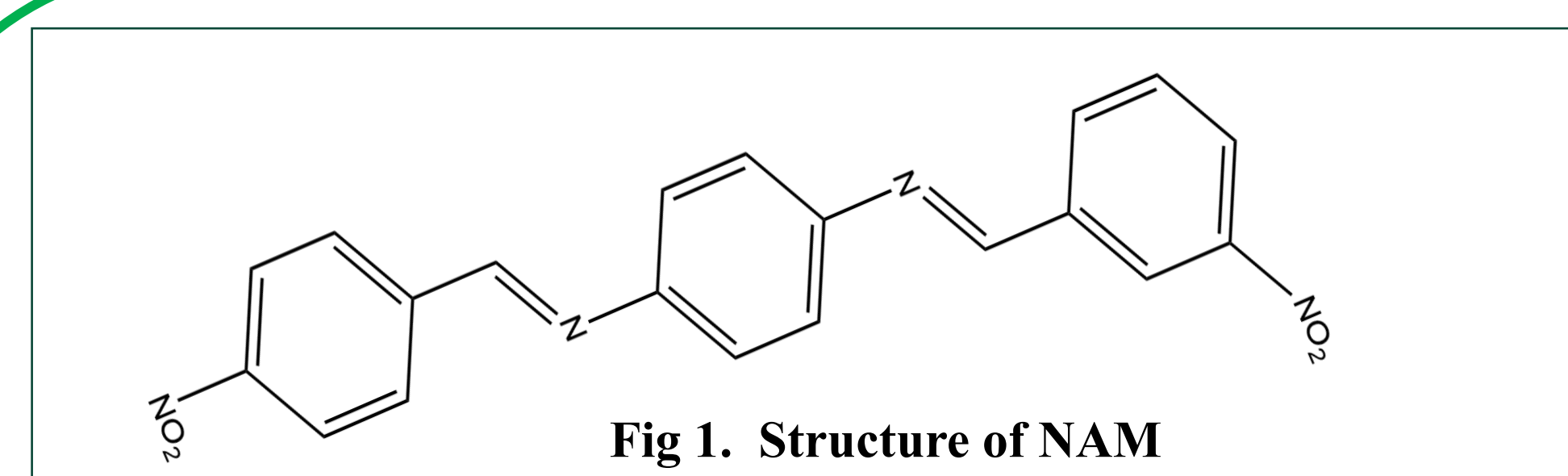


Time-Dependent Density Functional Theory
Functional: ω B97X-D
Basis set: 6-311++ G(d,p)
 $\omega = 1064$ nm
Gaussian 9 Software

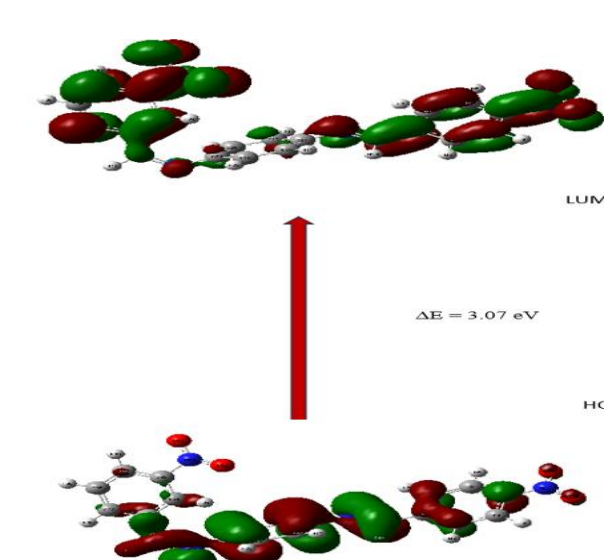
Key Parameters

- ❑ Dipole Moment
- ❑ Polarizability
- ❑ Hyperpolarizability

RESULT AND DISCUSSION



- ❑ Represents the most stable, lowest energy conformation of NAM
- ❑ Global Reactivity Measures



- ❑ HOMO–LUMO Gap (ΔE): 2.87 eV
- ❑ Gap decreases with solvent polarity $\rightarrow$ enhanced semiconducting and NLO properties.

Fig 3. Frontier molecular orbital and Energy gap of NAM

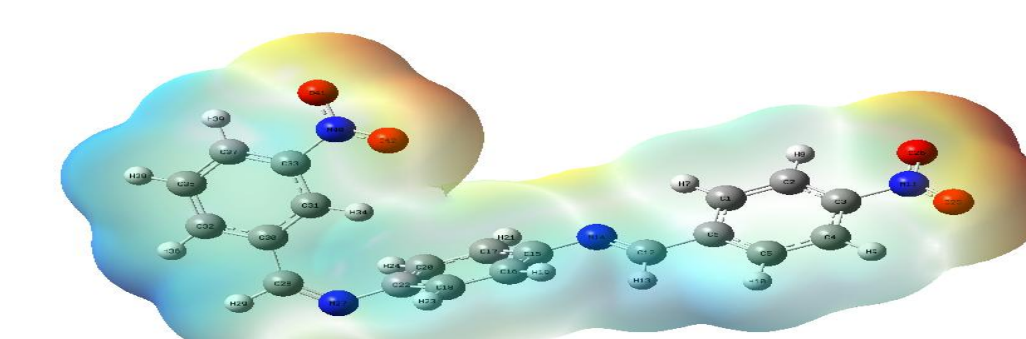
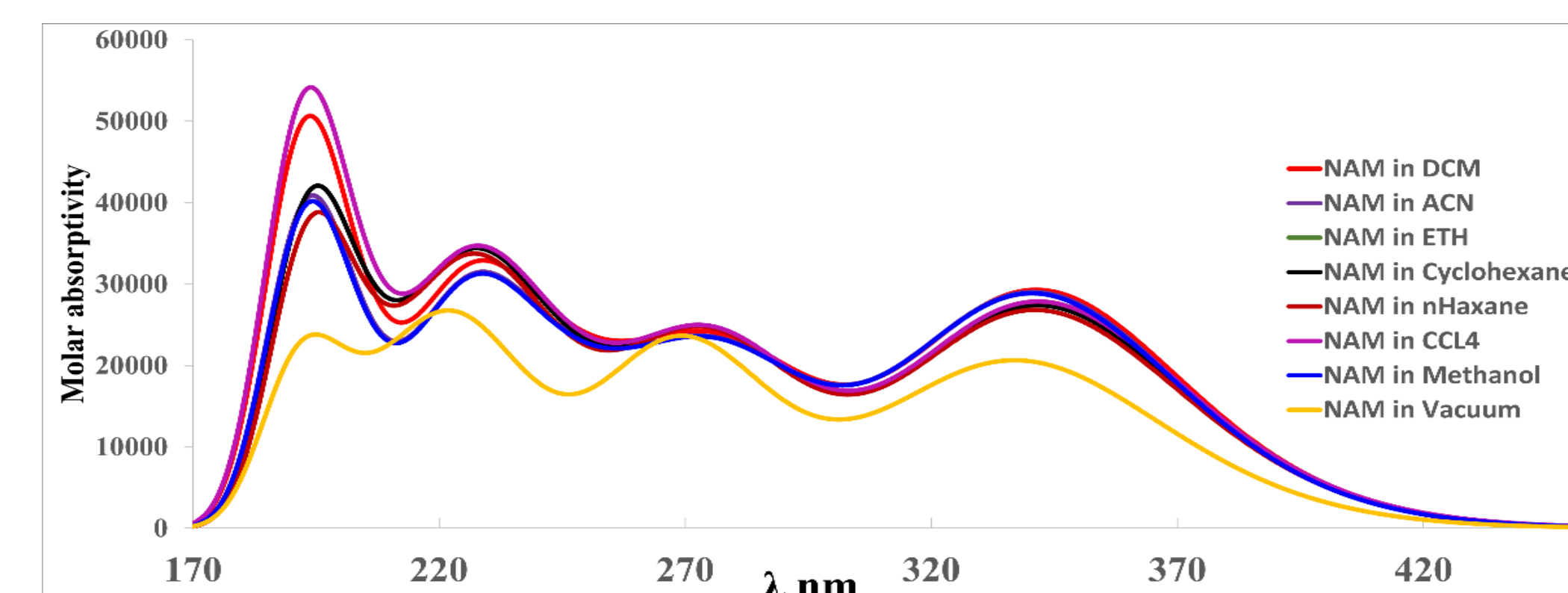


Fig 4. Structure of NAM



- ❑ Solvent-dependent shifts (red & blue shifts observed)
- ❑ $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ Transitions
- ❑ Light-Harvesting Efficiency (LHE): 61–79%

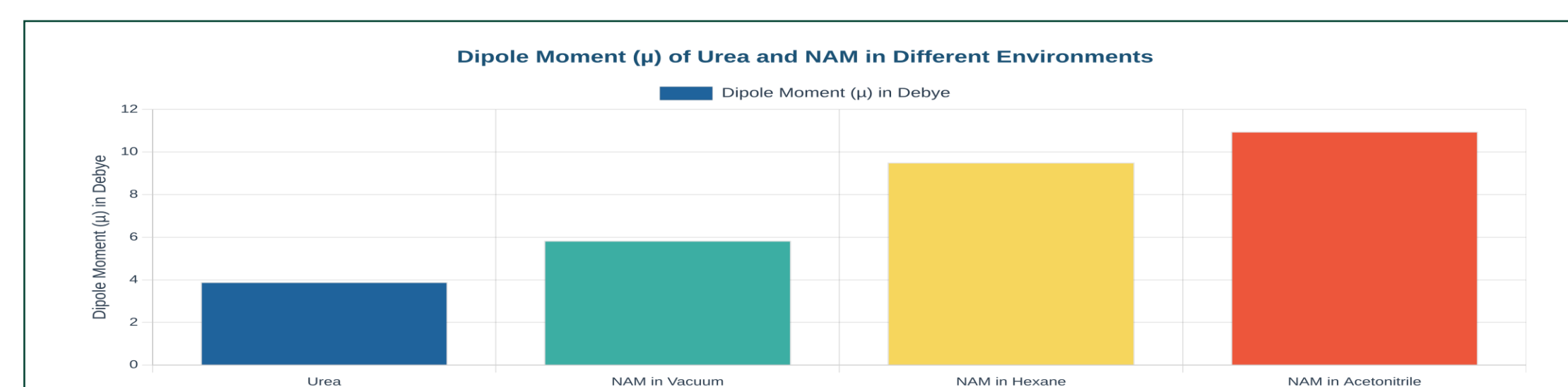
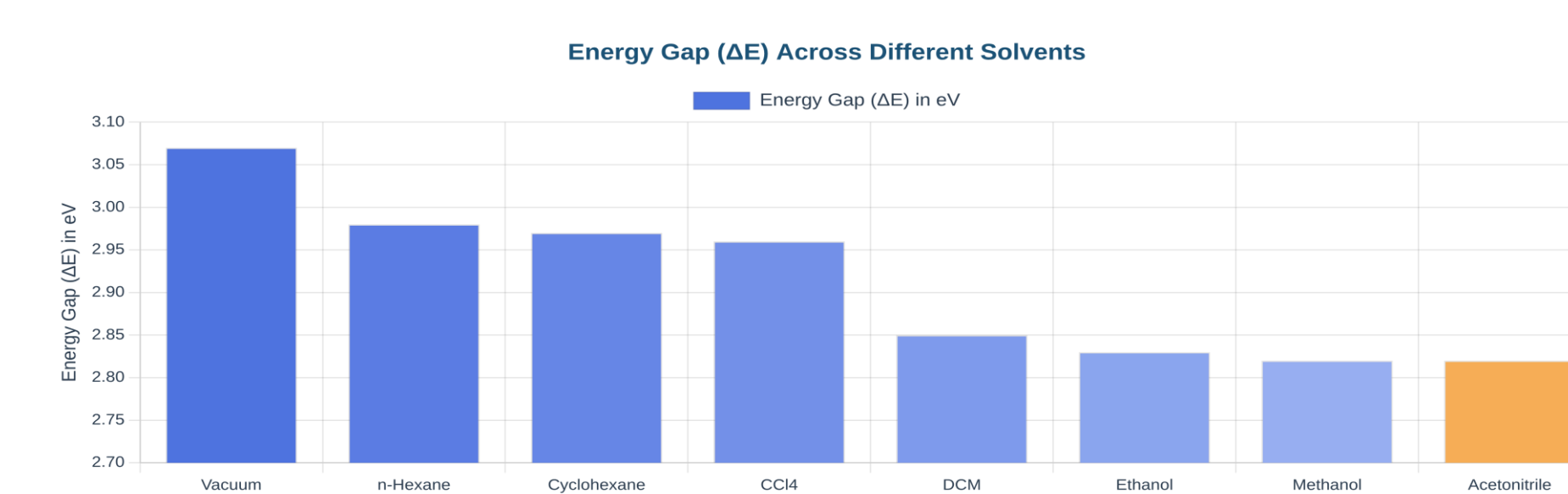
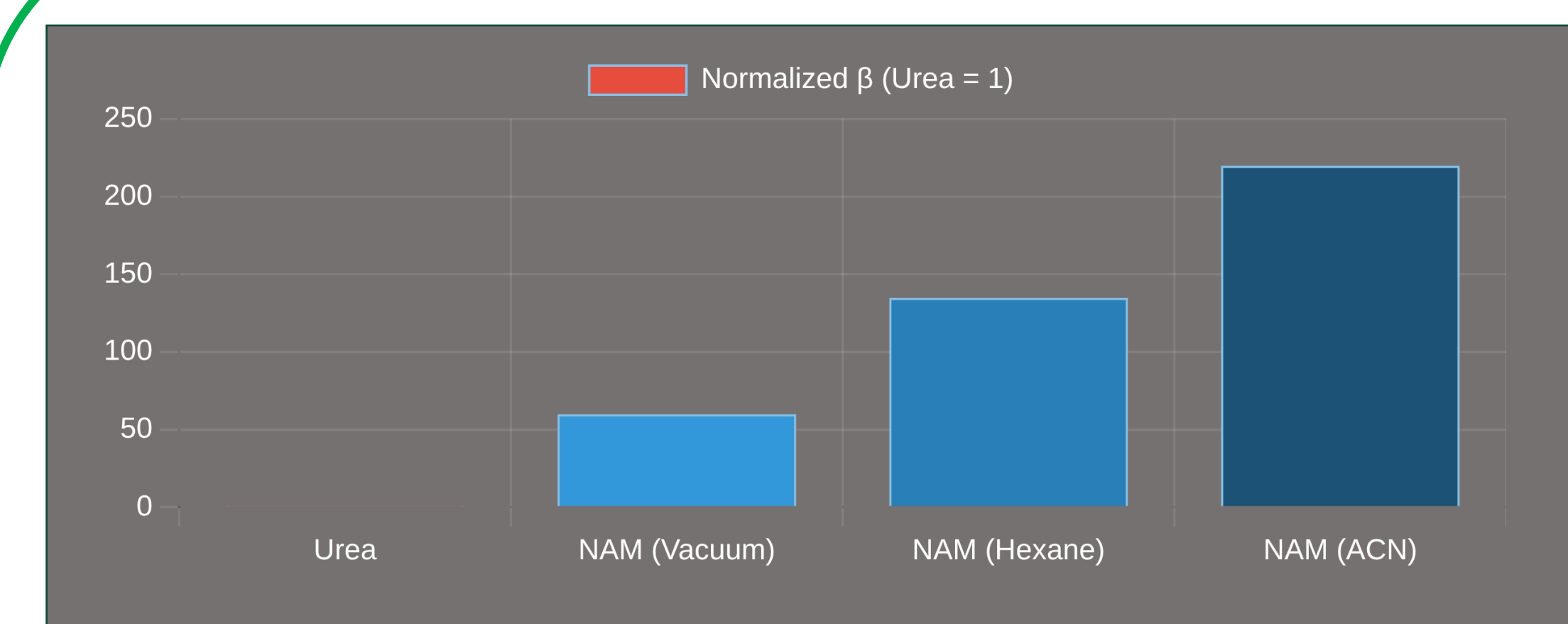
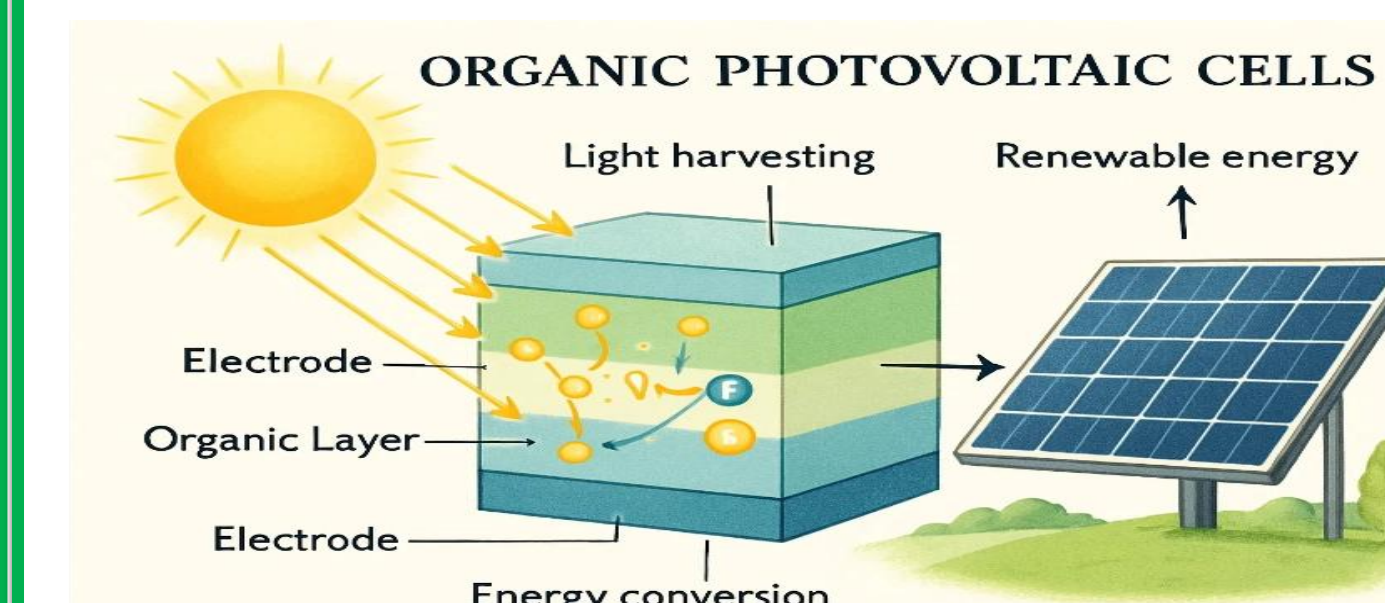


Fig 7. Dipole Moment of Urea and NAM in different solvents

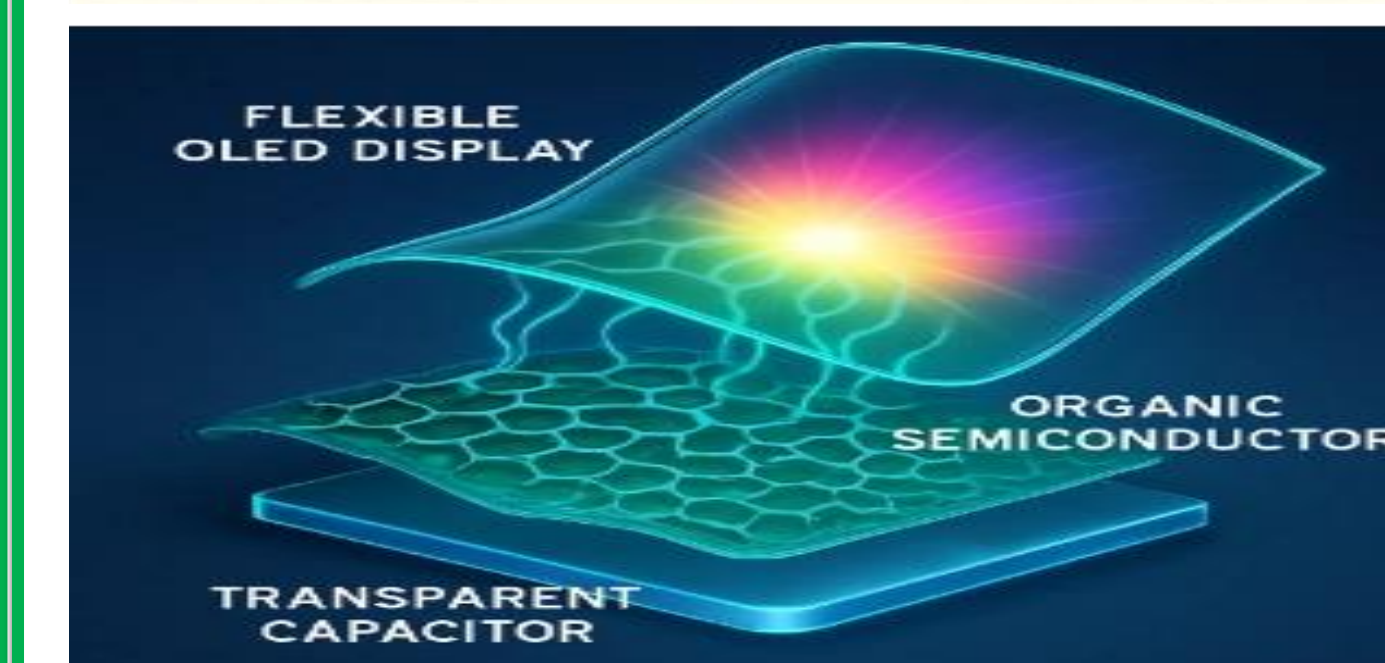


- ❑ Polarizability (α): ease of electron cloud distortion
- ❑ First hyperpolarizability (β) and Second hyperpolarizability (γ): 50 - 220 $\times$ higher than urea (reference)

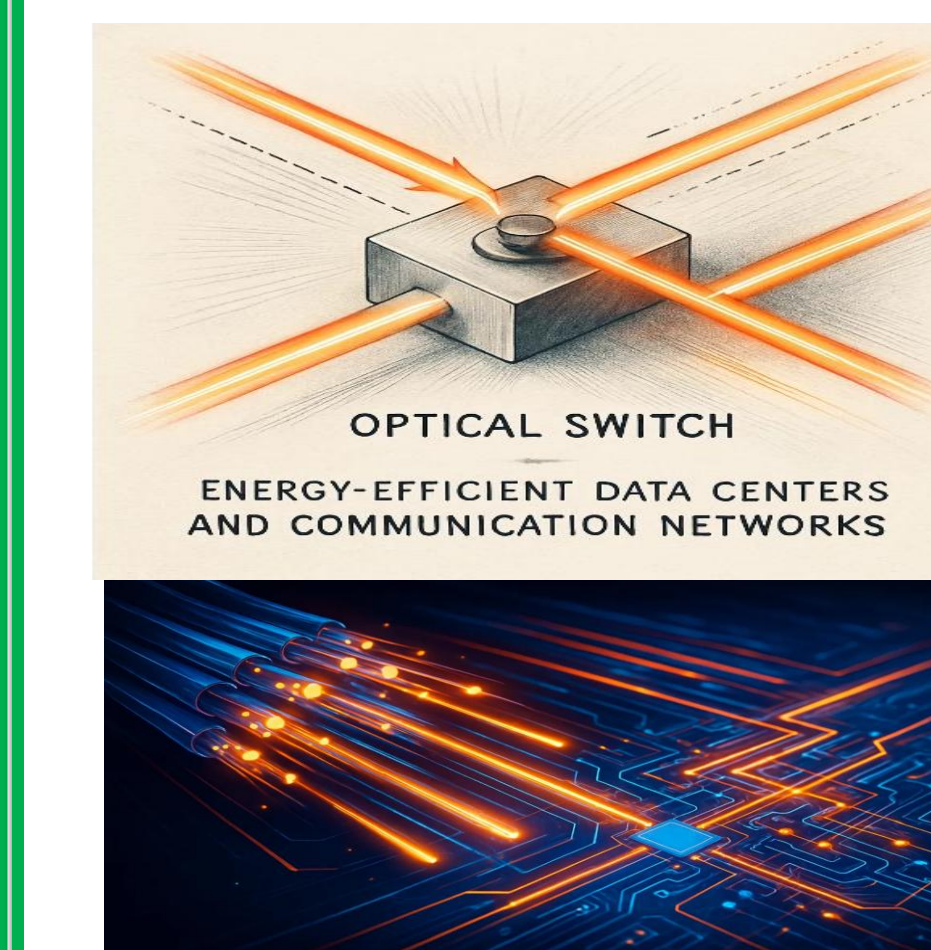
APPLICATION



NAM's high light-harvesting efficiency makes it an excellent candidate for organic photovoltaic cells, contributing to renewable energy solutions.



NAM's electronic structure and charge transport properties make it an excellent candidate for organic semiconductor applications in flexible electronics, OLEDs, and transistors.



NAM's exceptional nonlinear optical properties enable ultrafast electro-optic modulation for next-generation telecommunications infrastructure and can be incorporated into photonic devices for optical computing and signal processing, reducing energy consumption in data centers.

Conclusion

- ❑ NAM exhibits semiconducting and light-harvesting efficiencies in polar solvents
- ❑ NAM can be potentially applied in optics and optoelectronics
- ❑ NLO properties are up to 220 $\times$ enhanced as compared to urea (reference)

Future Directions

- ❑ Experimental validation of computational predictions

References

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- 2.International Energy Agency (IEA). (2023). *Energy and climate change*.

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