

COMPUTATIONAL CHEMISTRY METHODS TO IDENTIFY EFFICIENT COUMARIN DYES FOR SOLAR CELLS



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Introduction

- Research on designing solar cells for low-cost sustainable energy production, reduction of dependency on finite fossil fuels and its environmental impact is a continuous focus.
- Using dye-sensitized solar cells, hydrogen fuel and oxygen can be obtained by photocatalytic water splitting [1].
- Hydrogen is an energy carrier with high energy density. When burned, it gives clean energy & water as opposed to fossil fuels to meet the UN Sustainable Development Goal #7.
- Coumarin dyes are popular due to their fluorescent properties and excellent stability in the sun over time.
- However, the limitation with coumarin dyes is that they absorb light in the visible region but weakly over 700 nm, making it a challenge to extend their photoresponse in the visible region [2].
- In this work, we studied eight new variants of C343 coumarin dye using computational chemistry techniques based on density functional theory and a solar cell capacitance simulator by changing the chromophoric system and modulating the electric field.

Why is this work Important?

It allows for the evaluation of the suitability of novel coumarin dyes for dye-sensitized solar cells (DSSC) towards affordable & clean energy-Hydrogen fuel production thereby meeting the UN SDG 7.

References

- [1] Y. Li, D. Bahamon, M. Sinnokrot, K. Al-Ali, G. Palmisano and L. Vega, J. Photochem. Photobiol, 2021, 49, 1-11
- [2] M. M. Waskasi, S. M. Hashemianzadeh, Mostajabi Sarhangi, A. P. Harzandi, Energy Convers. Manag. 2012, 62, 154-164.

Computational Methods

Derivation of C343 modified dyes

Molecular modelling of C343, C343-1 to C343-8 using Avogadro

Ground state optimization in gas & water using B3LYP functional & 6-311G(d) basis set: Computations were carried out using ORCA 5.0

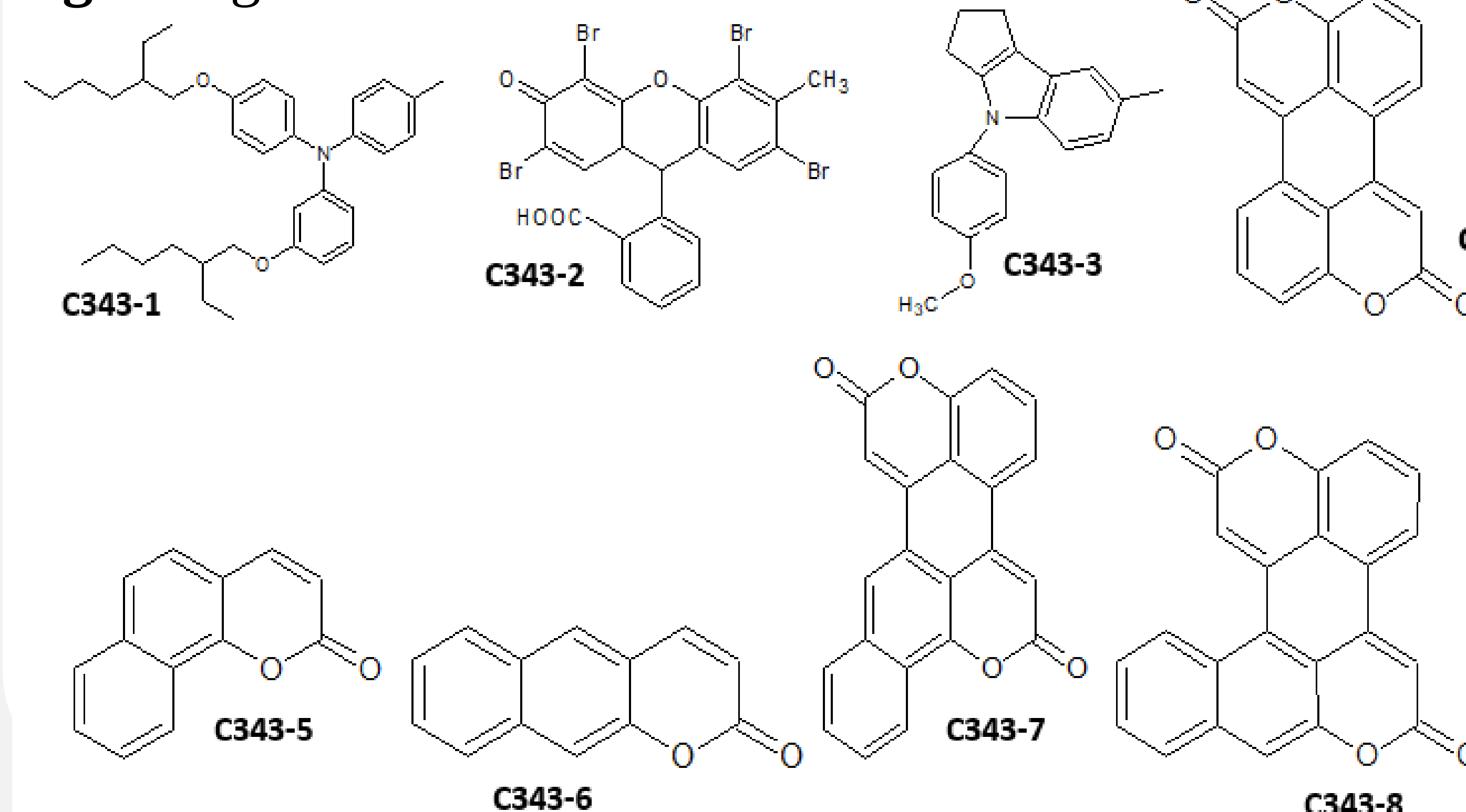
TD-DFT calculations (excitation energies, oscillator strength, absorption spectra, dipole moment, polarizability)

Photovoltaic properties determination using Solar Cell Capacitance Simulator with reference to C343 dye

Table 1: C343 reference properties

C343	Band gap (eV)	Max absorption Wavelength (nm)
Gas	3.60	344.2
Water	3.07	403.7

Fig.1: Eight coumarin derivatives of C343



Sunlight

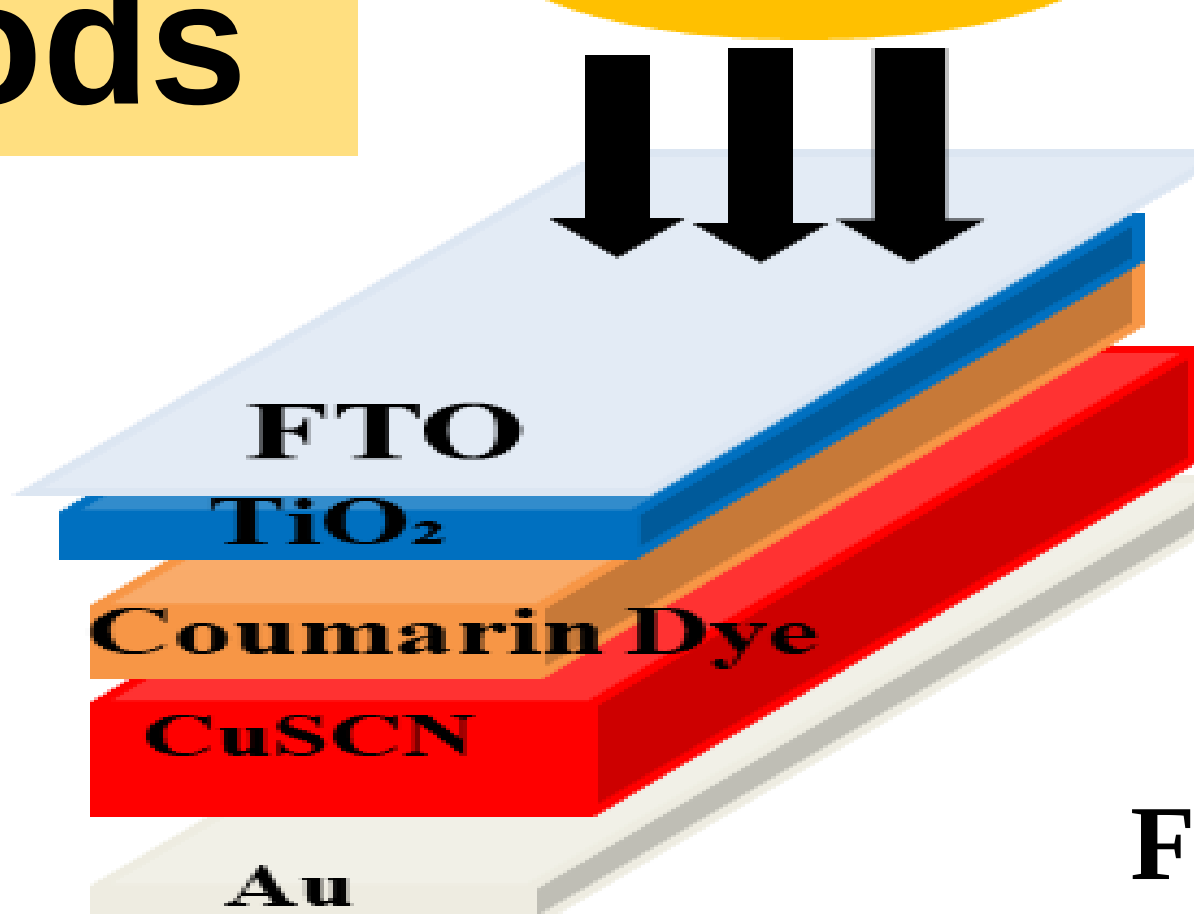


Fig.2: Schematic of DSSC for photovoltaic properties analysis

Electric fields: 0, 10, 20, 30, 40 and 50 $\times 10^{-4}$ a.u applied to most promising dye

TD-DFT calculations (excitation energies, oscillator strength, absorption spectra, dipole moment, polarizability)

Results...

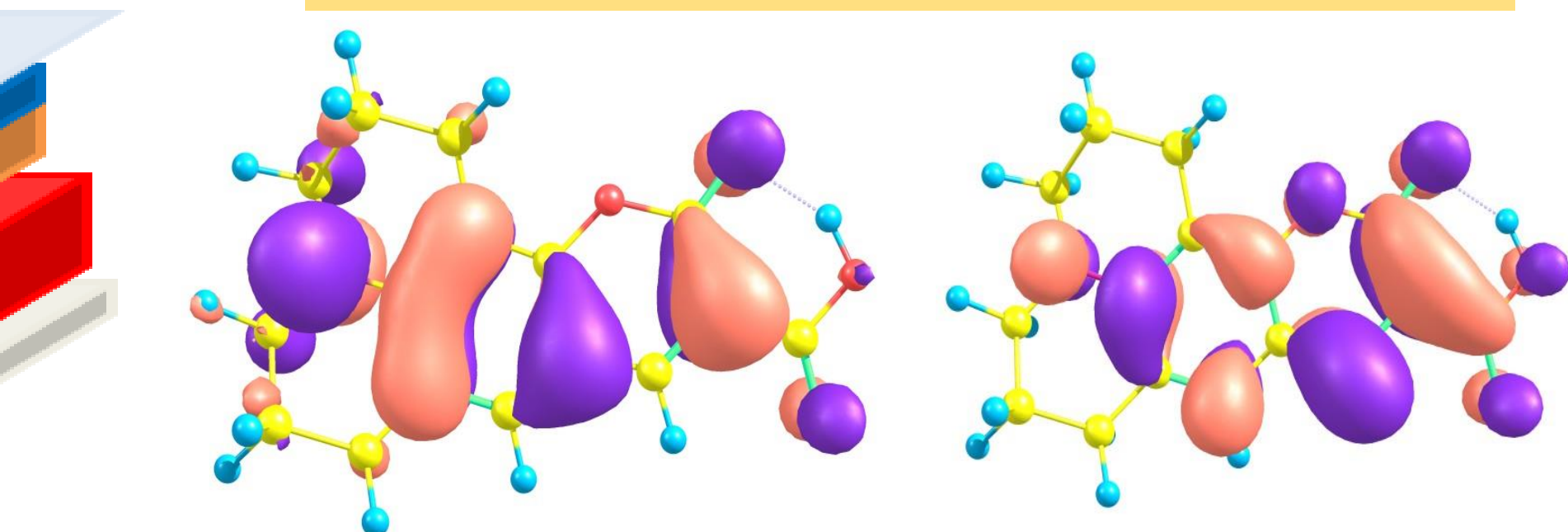


Fig.3: HOMO and LUMO of C343 dye in gas

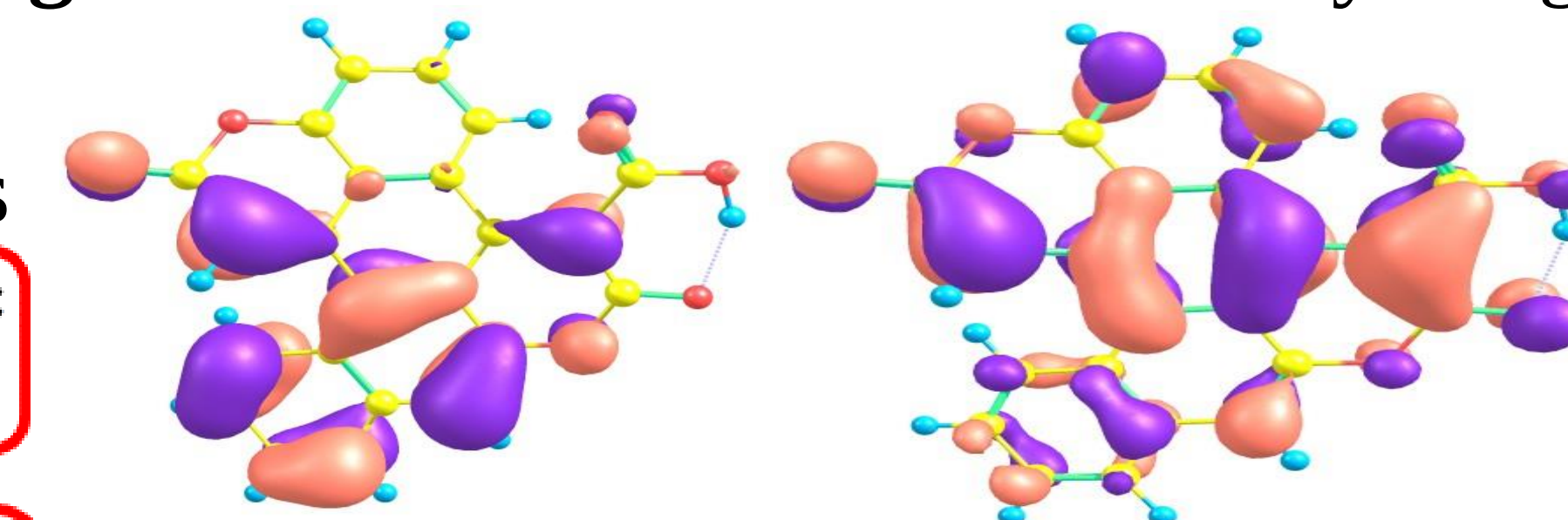


Fig.4: HOMO and LUMO of C343-8 dye in gas

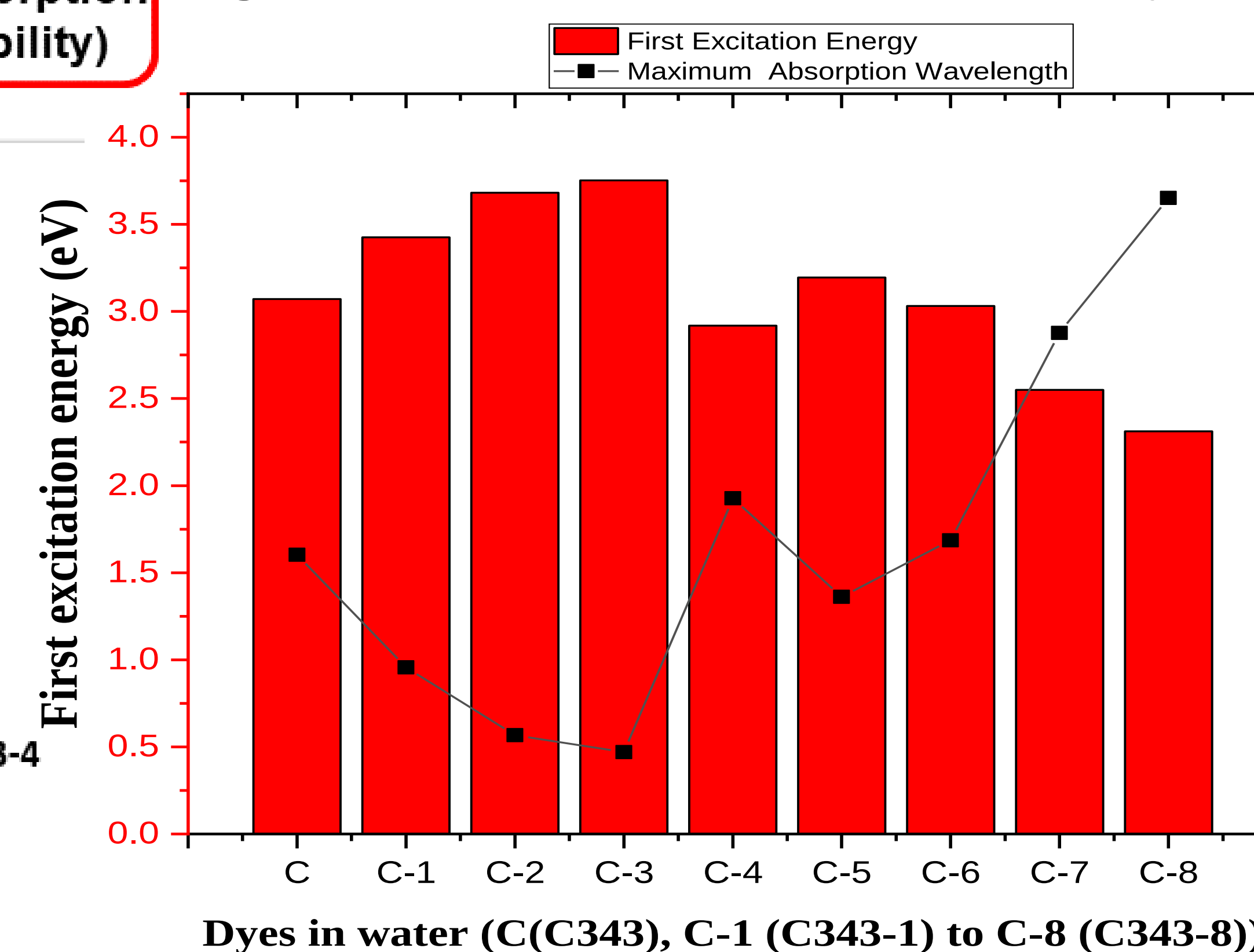


Fig.5: First Excitation Vs Max Absorption Wavelength

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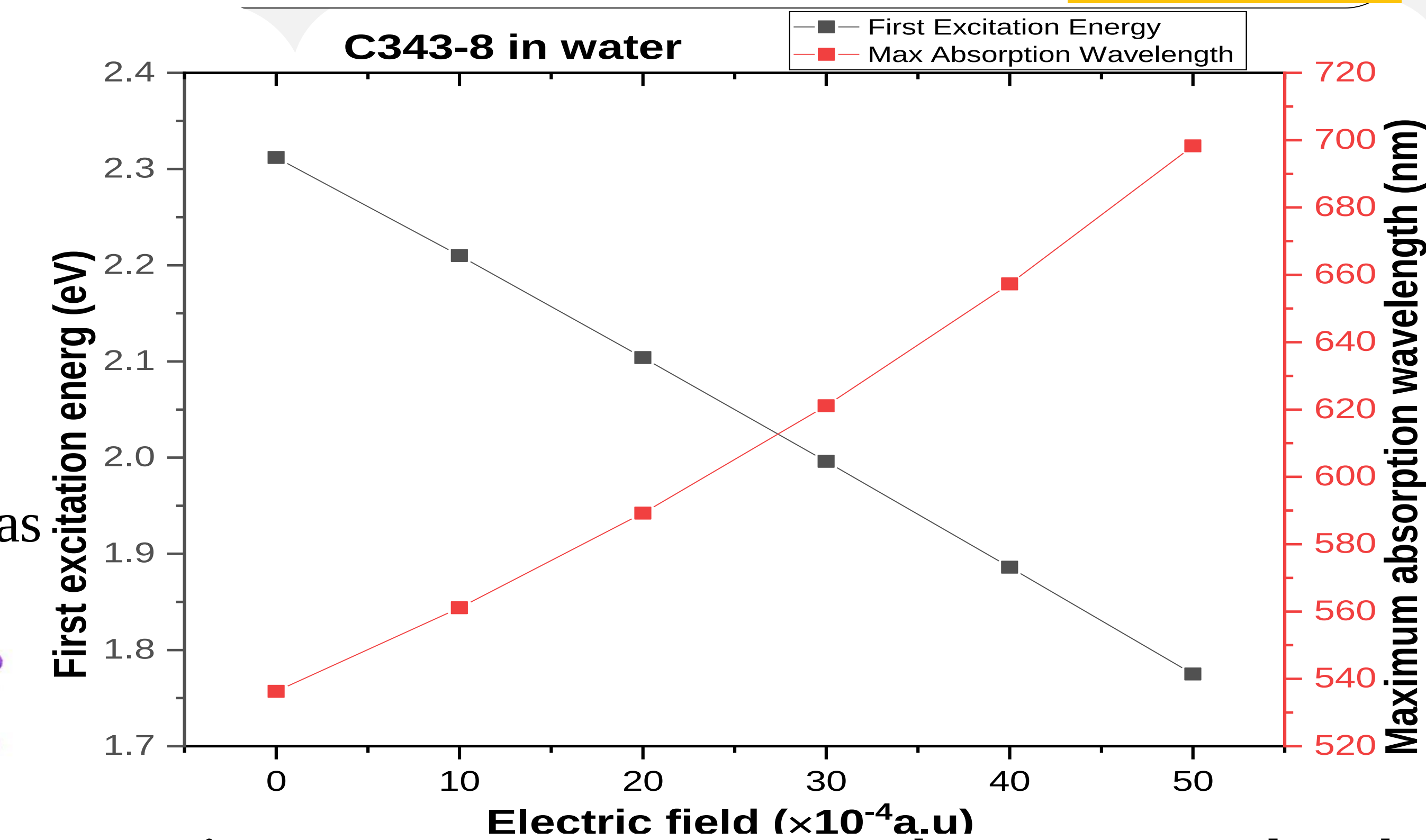


Fig.6: First Excitation Vs Max Absorption Wavelength

Table 2. Photovoltaic parameters obtained in gas phase

Dye	V _{oc} (eV)	J _{sc} (mAcm ⁻²)	FF(%)	Efficiency(%)
C343	1.16	586.30	87.51	0.59
C343-8	1.15	4.69	72.93	3.94

Table 3. Photovoltaic parameters in water

Dye	V _{oc} (eV)	J _{sc} (mAcm ⁻²)	FF(%)	Efficiency(%)
C343	1.15	1.12	79.60	1.02
C343-8	1.14	12.18	74.78	10.36

Conclusions

- The findings indicate that C343-8 derivative is more effective (compared to C343-Table 1) with:
 - band gap of 2.24 eV in gas & 1.78 eV in water
 - maximum absorption wavelength of 553.9 nm in gas and 698.3 nm in water
 - power conversion efficiency of 3.94 in gas and 10.36 in water
- This gives enhanced light absorbing abilities to the coumarin dye which therefore promotes hydrogen production by dye sensitized water splitting a step further towards its widespread commercial application which meets UN-SDG 7.