KU LEUVEN

Quantitative predictions of photochemistry from excited state decay rate calculations

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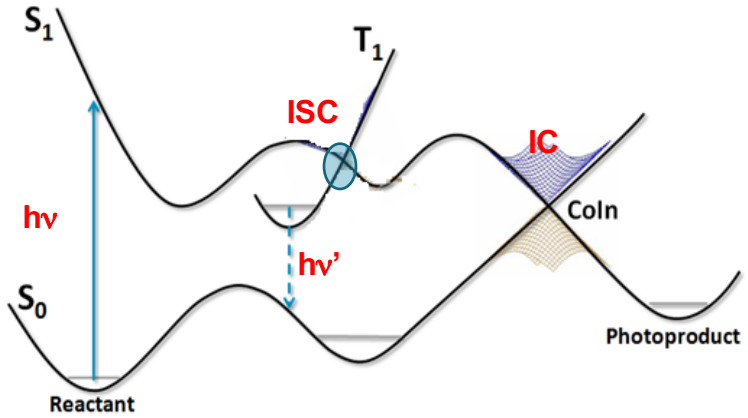
Computational Photochemistry

1. **Photophysics & Adiabatic chemistry**
2. **Non-adiabatic photochemistry**

} → **Quantum chemistry**

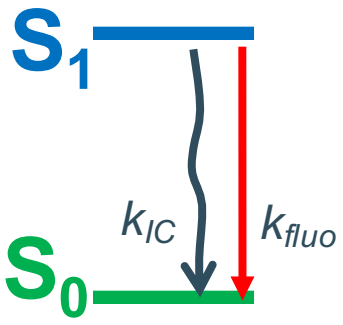
3. **Time-resolved information & Quantum yields → 1. Dynamic approach**

2. Static approach: Calculation of rate constants from first principles.



❖ Static approach:[1]

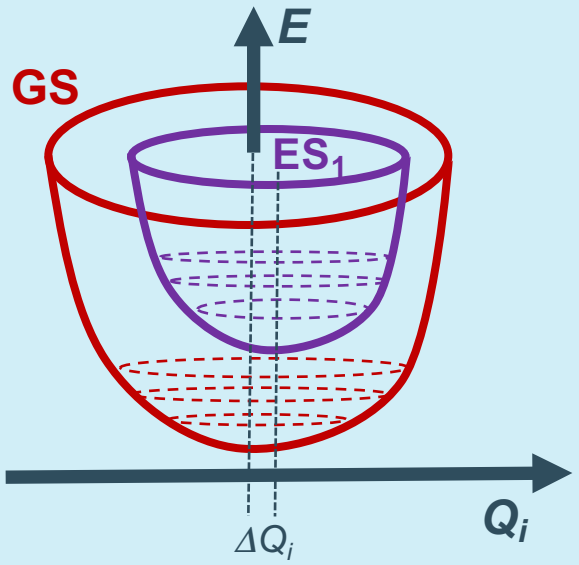
- Benchmark quantum chemical methods for the ES: Geometries, ES energies, gradients, vibronic, SOCs, NACs, etc
- Use diverse ES decay rate formalisms providing access to radiative (k_r) and nonradiative rates (k_{nr})
- Develop realistic kinetic models and derive of the kinetic master equations:



[1] *See also work by Marian, Penfold, Shuai, Peng, etc.*

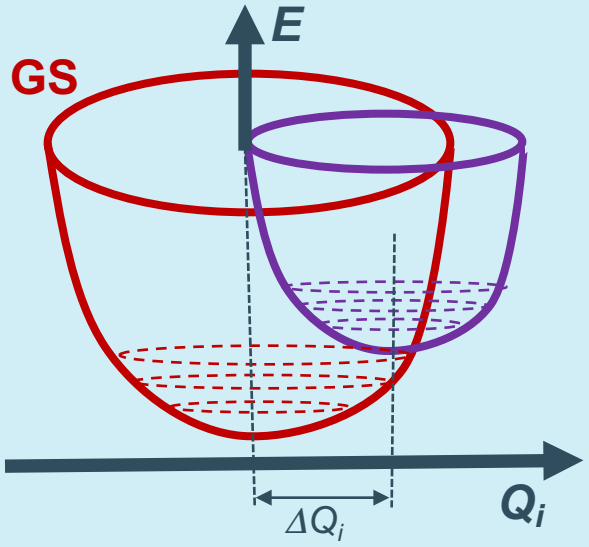
Challenge: Non-radiative deactivation decay rates

Weak coupling regime



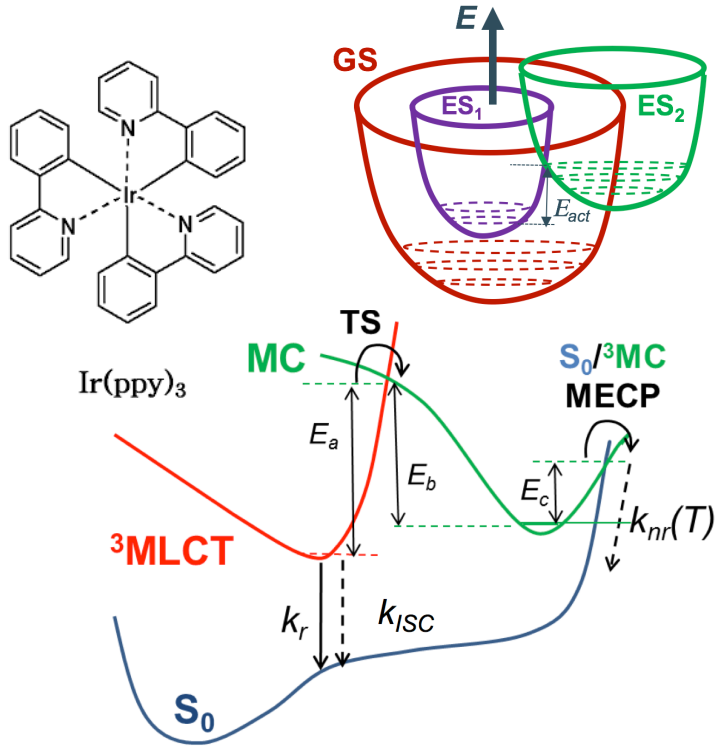
Rigid molecules /
Fluorophores / Phosphors

Strong coupling regime



Non-adiabatic
photochemistry

Predicting PLQY of phosphors:[1]



Take home message: An exploration of the ES PES is needed!

[1] *X. Zhang, D. Jacquemin, Q. Peng, Z. Shuai, D. Escudero,* ***J. Phys. Chem. C,*** 122, 6340 (2018)

Excited state decay rates: Thermal vibration correlation function (TVCF) theory

❑ k_{IC} and k_r are computed with **Thermal Vibration Correlation Function** (TVCF)[1] theory:

- **k_{IC} :** Fermi-Golden rule expression

$$k_{\mathrm{ic}} = \frac{2\pi}{\hbar}|H'_{\mathrm{fi}}|^2\delta(E_{\mathrm{fi}} + E_{\mathrm{f}v_{\mathrm{f}}} - E_{\mathrm{i}v_{\mathrm{i}}}) \qquad \text{where: } H'_{\mathrm{fi}} = -\hbar^2\sum_l \langle \Phi_{\mathrm{f}}\Theta_{\mathrm{f}v_{\mathrm{f}}}|\frac{\partial\Phi_{\mathrm{i}}}{\partial Q_{\mathrm{f}l}}\frac{\partial\Theta_{\mathrm{i}v_{\mathrm{i}}}}{\partial Q_{\mathrm{f}l}}\rangle$$

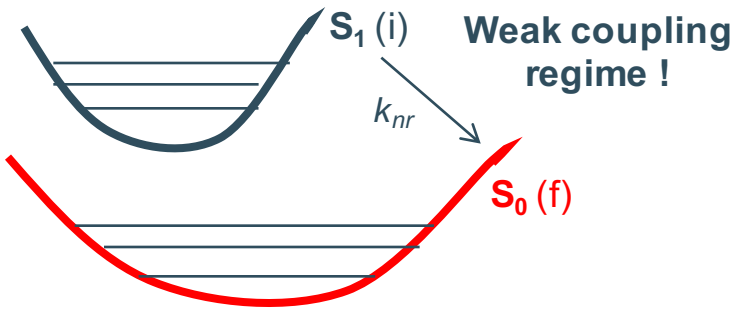
Applying Condon Approximation:

$$k_{ic} = \frac{2\pi}{\hbar}\sum_{kl} R_{kl}Z_{iv}^{-1}\sum_{v_{\mathrm{i}},v_{\mathrm{f}}} \mathrm{e}^{-\beta E_{\mathrm{i}v_{\mathrm{i}}}}P_{kl}\delta(E_{\mathrm{fi}} + E_{\mathrm{f}v_{\mathrm{f}}} - E_{\mathrm{i}v_{\mathrm{i}}}) \qquad \text{where } R_{kl} = \langle\Phi_{\mathrm{f}}|\hat{P}_{\mathrm{f}k}|\Phi_{\mathrm{i}}\rangle\langle\Phi_{\mathrm{i}}|\hat{P}_{\mathrm{f}l}|\Phi_{\mathrm{f}}\rangle$$
$$P_{kl} = \langle\Theta_{\mathrm{f}v_{\mathrm{f}}}|\hat{P}_{\mathrm{f}k}|\Theta_{\mathrm{i}v_{\mathrm{i}}}\rangle\langle\Theta_{\mathrm{i}v_{\mathrm{i}}}|\hat{P}_{\mathrm{f}l}|\Theta_{\mathrm{f}v_{\mathrm{f}}}\rangle$$

The delta function is Fourier transformed:

$$k_{ic} = \frac{1}{\hbar^2}\sum_{kl} R_{kl}\int_{-\infty}^{\infty}\mathrm{d}t\,[\mathrm{e}^{\mathrm{i}\omega_{\mathrm{if}}t}Z_{\mathrm{i}v}^{-1}\rho_{\mathrm{ic},kl}(t,T)]$$

TVCF for IC



MOMAP: Multidimensional harmonic oscillator model coupled to quantum chemical calculations where displacements, distortions and Duschinsky rotations effects[2]

We need: GS and ES geometries, 2nd derivatives, NACs, etc.

- **k_r :** Einstein spontaneous emission

$$k_r = \frac{8\pi^2\nu_{fi}^3}{3\varepsilon_0\hbar c^3}\mu_{fi}^2 \approx \frac{fv_{fi}^2}{1.5}$$

Or by integrating the computed emission spectra (by TVCF):

$$k_r = \int_0^\infty \sigma_{em}(\omega)d\omega = \int_0^\infty \sigma_{em}^{FC}(\omega)d\omega + \sum_k \sigma_{em,k}^{FC/HT}(\omega)d\omega + \sum_{k,l}\sigma_{em,kl}^{HT}(\omega)d\omega$$

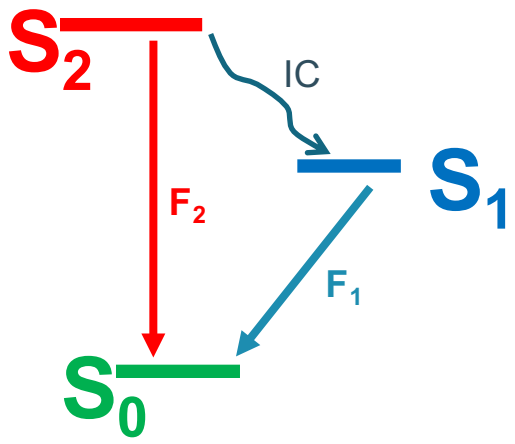
$$\vec{\mu}_{\mathrm{fi}} = \vec{\mu}_0 + \sum_k \vec{\mu}_k Q_k + \sum_{k,l}\vec{\mu}_{kl}Q_kQ_l$$

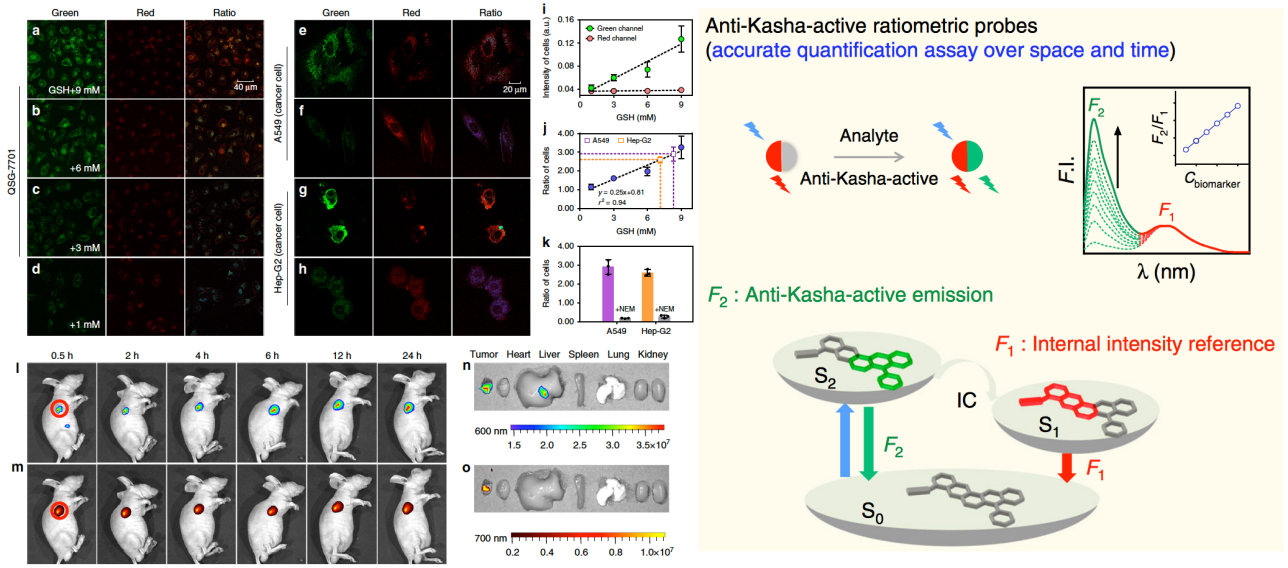
[1] *Shuai et al.,* ***J. Phys. Chem. A,*** 114, 7817 (2010)

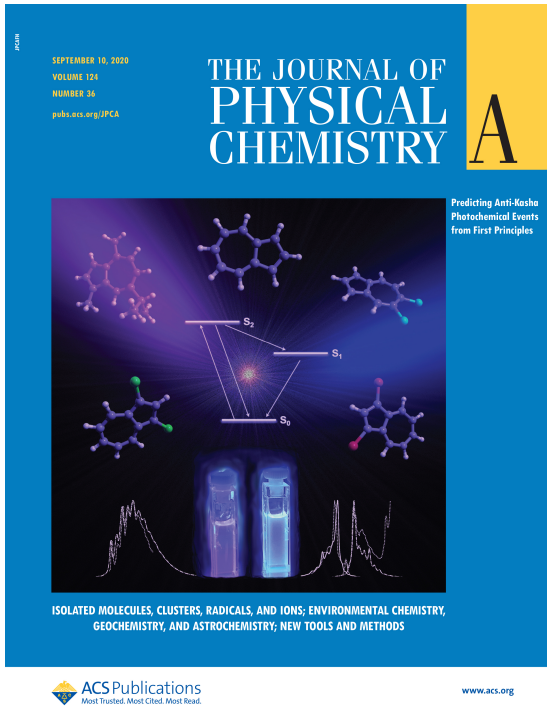
[2] MOMAP, Shuai group: Beijing, CN, 2014, http://www.shuaigroup.net/

Outline

- Computational protocol to predict anti-Kasha emissions:



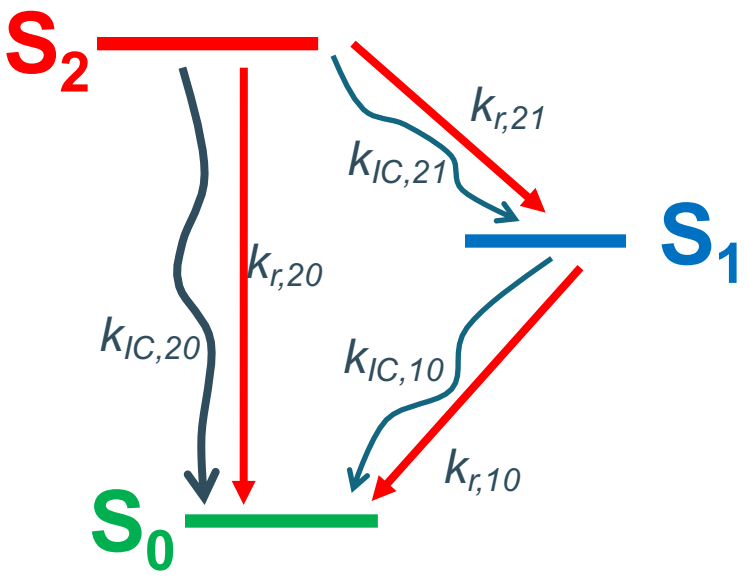




- Computational protocol to predict the temperature-dependent photoluminescence lifetimes and yields of phosphors.

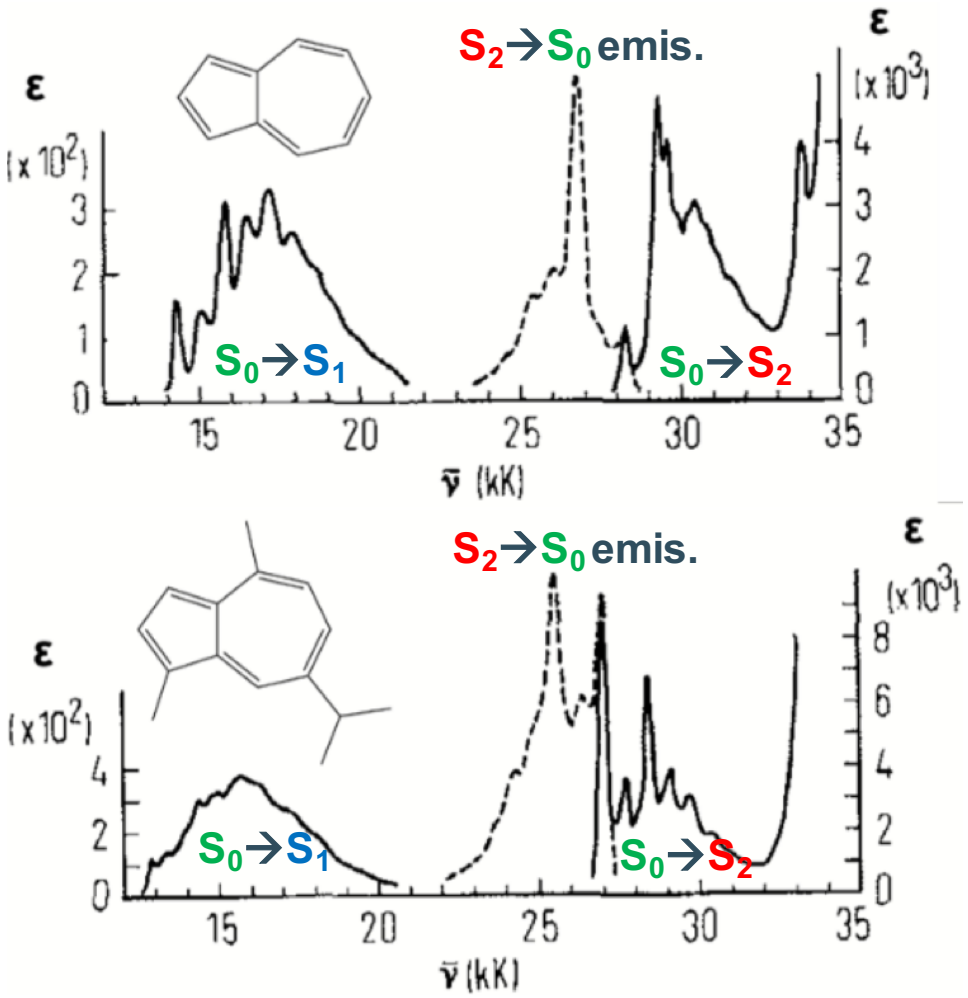
Shi et al., ***Nature Communications,*** 11, 793 (2020)

Kinetic model for anti-Kasha photoluminescence: azulenes



$$\phi_{20} = k_{r,20} * \tau_2 \approx \frac{k_{r,20}}{k_{r,20} + k_{ic,21}}$$

$$\phi_{10} \approx \frac{k_{r,10}}{k_{r,10} + k_{ic,10}} * \frac{k_{ic,21}}{k_{r,20} + k_{ic,21}}$$



Murata et al., ***Berichte der Bunsengesellschaft für Phys. Chemie***, *76*, 117 (1972)

Azulene's anti-Kasha photoluminescence: benchmarking electronic structure methods

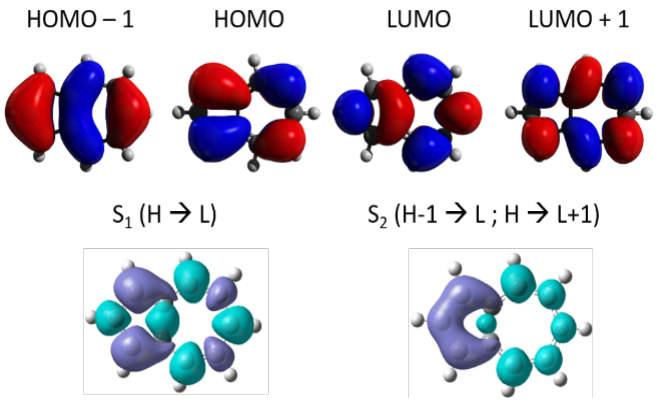
- **TD-PBE0/6-31G(d)** and **ADC(2)/def2-TZVP** (between parentheses) results:

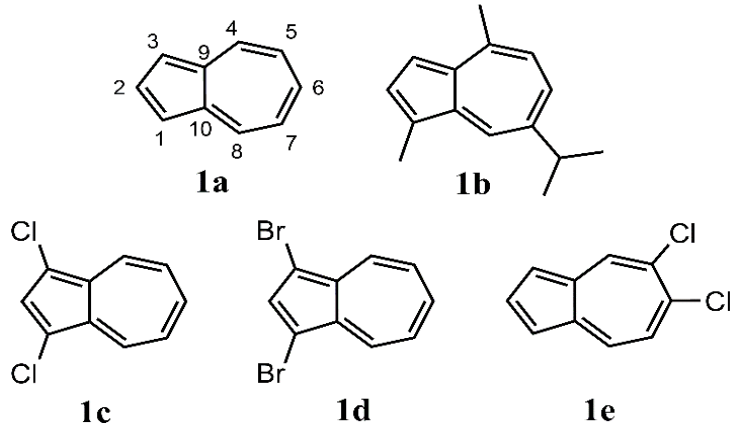
$S_0 \rightarrow S_1$:

	E_v (eV)	*f* (au)	$E^{0\text{-}0}$ (eV)	Exp. $E^{0\text{-}0}$ (eV)[1]
1a	**2.47** (**2.24**)	**0.008** (**0.009**)	**2.04** (**1.81**)	1.77

$S_0 \rightarrow S_2$:

E_v (eV)	*f* (au)	$E^{0\text{-}0}$ (eV)	Exp. $E^{0\text{-}0}$ (eV)[1]
3.77 (**3.85**)	**0.002** (**0.005**)	**3.61** (**3.66**)	3.50



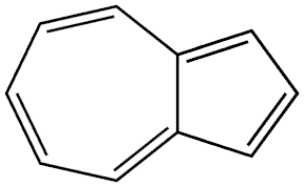


K. Veys

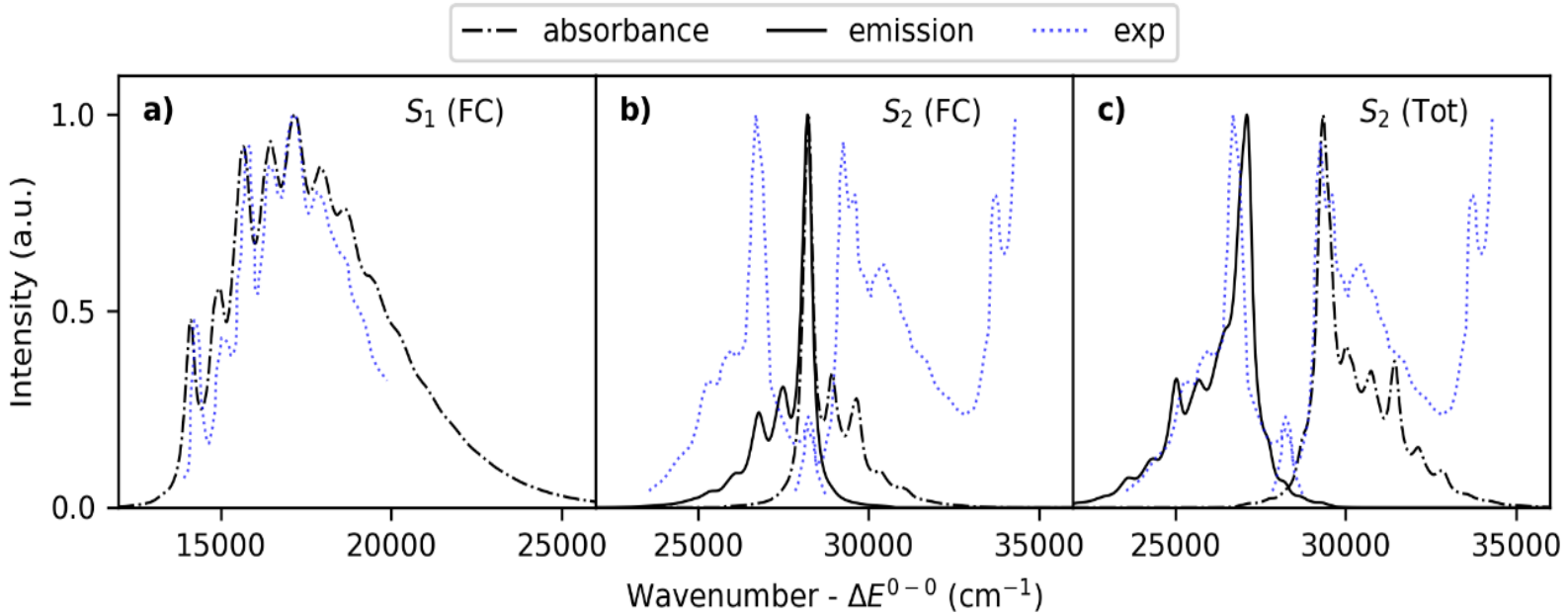
K. Veys, D. Escudero, ***J. Phys. Chem A****, 124, 7228 (2020)*
[1]*Griesser,* ***Chem. Phys.,*** 52, 117 (1980)

Azulene's anti-Kasha photoluminescence: UV-Vis spectra

❑ **TVCF absorption and emission spectra:**



1a

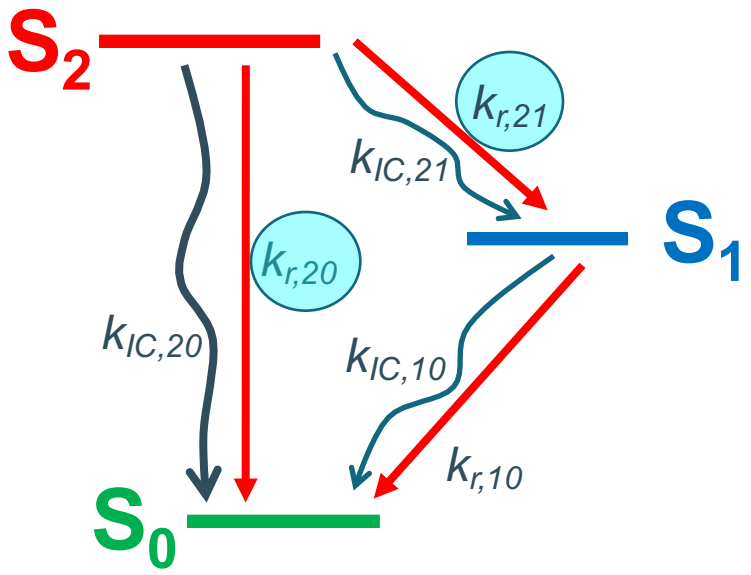


Based on:
1) ADC(2)/def2-TZVP energy gaps
2) ADC(2)/def2-TZVP TDMs
3) TD-PBE0/6-31G(d) geometries and Hessian calculations

HT effects are important for the S_2 band of **1a**

K. Veys, D. Escudero, ***J. Phys. Chem A****, 124, 7228 (2020)*
Griesser, ***Chem. Phys.,*** 52, 117 (1980)

Azulene's anti-Kasha photoluminescence: k_r calculations



$$k_{r,20} >> k_{r,21}$$

$$k_r = \frac{8\pi^2 \nu_{fi}^3}{3\varepsilon_0 \hbar c^3} \mu_{fi}^2 \approx \frac{f \nu_{fi}^2}{1.5}$$

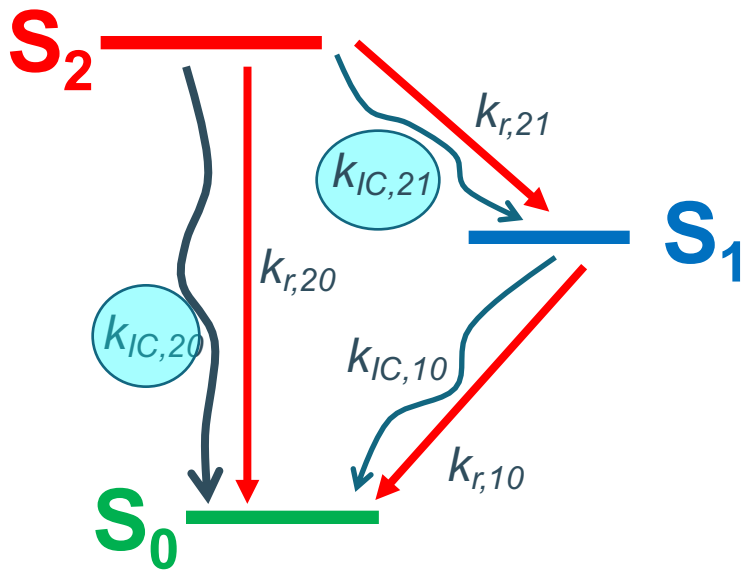
- Computed k_r values with TVCF (experimental values between parentheses)[1,2]:

	k_r ($\times 10^7$ s^{-1})	
	$S_1 \rightarrow S_0$	$S_2 \rightarrow S_0$
1a	0.16	2.7 (2.3±0.1)
1b	0.12	1.7 (3.2±0.4)
1c	0.15	2.5 (3.6±0.1)
1d	0.20	2.7 (3.5)
1e	0.12	1.2 (2.4)

Based on:
1) ADC(2)/def2-TZVP energy gaps
2) ADC(2)/def2-TZVP TDMs
3) TD-PBE0/6-31G(d) geometries and Hessian calculations

[1]Murata et al., ***Berichte der Bunsengesellschaft für Phys. Chemie***, *76*, 117 (1972)
[2]Griesser, ***Chem. Phys.,*** 52, 117 (1980)

Azulene's anti-Kasha photoluminescence: k_{nr} calculations



$$k_{IC,21} >>> k_{IC,20}$$

$$k_{IC} = \left(\frac{2\pi}{\hbar}\right) H^2 * FCWD$$

$$FCWD = \frac{1}{\sqrt{4\pi\lambda RT}} \exp\left(-\frac{(\Delta G + \lambda)^2}{4\pi\lambda RT}\right)$$

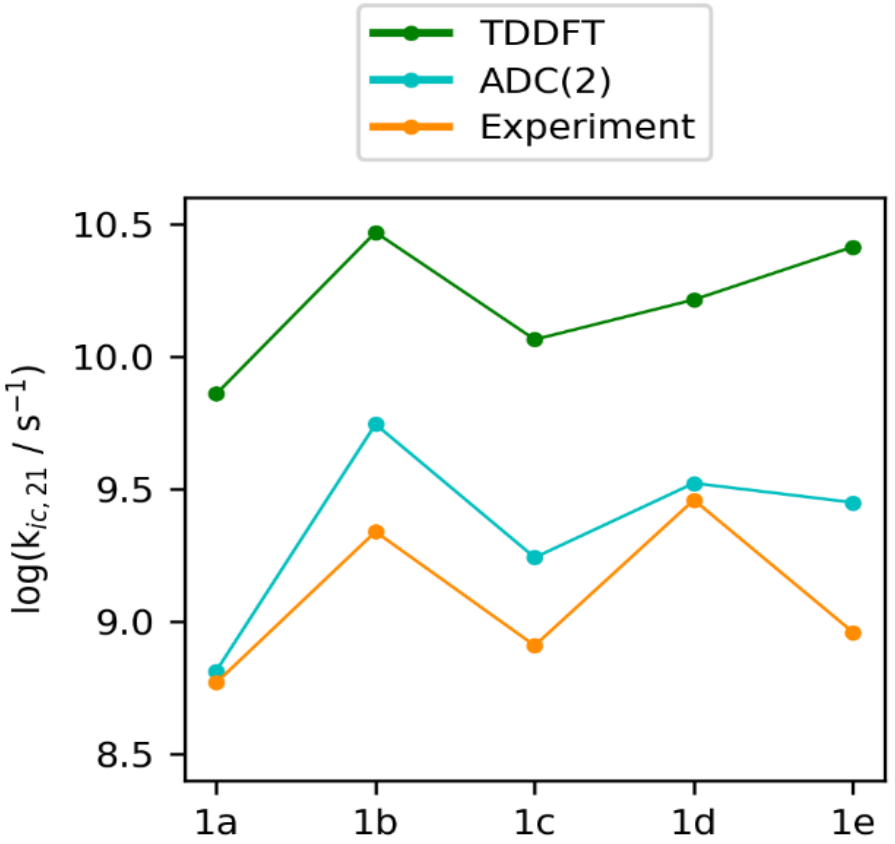
- Computed k_{IC} values with TVCF (experimental values between parentheses)[1,2]:

	k_{ic} (s^{-1})	
	$S_1 \rightarrow S_0$	$S_2 \rightarrow S_1$
1a	1.9×10^{11}	6.3×10^{8} ($5.3\pm1.2\times10^{8}$)
1b	6.7×10^{11}	5.5×10^{9} ($2.1\pm0.1\times10^{9}$)
1c	7.8×10^{11}	1.7×10^{9} ($7.0\pm1.2\times10^{8}$)
1d	1.0×10^{12}	3.3×10^{9} (2.9×10^{9})
1e	4.6×10^{11}	2.7×10^{9} (9.0×10^{8})

Based on:
1) ADC(2)/def2-TZVP energy gaps
2) ADC(2)/def2-TZVP NACs for $S_1 \rightarrow S_0$ and $S_2 \rightarrow S_0$
3) CIS/6-31G(d) NACs for $S_2 \rightarrow S_1$
4) TD-PBE0/6-31G(d) Hessian calculations

[1]Murata et al., ***Berichte der Bunsengesellschaft für Phys. Chemie***, *76*, 117 (1972)
[2]Griesser, ***Chem. Phys.,*** 52, 117 (1980)

Azulene's anti-Kasha photoluminescence: k_{nr} calculations



$$k_{IC} = \left(\frac{2\pi}{\hbar}\right) H^2 * FCWD$$

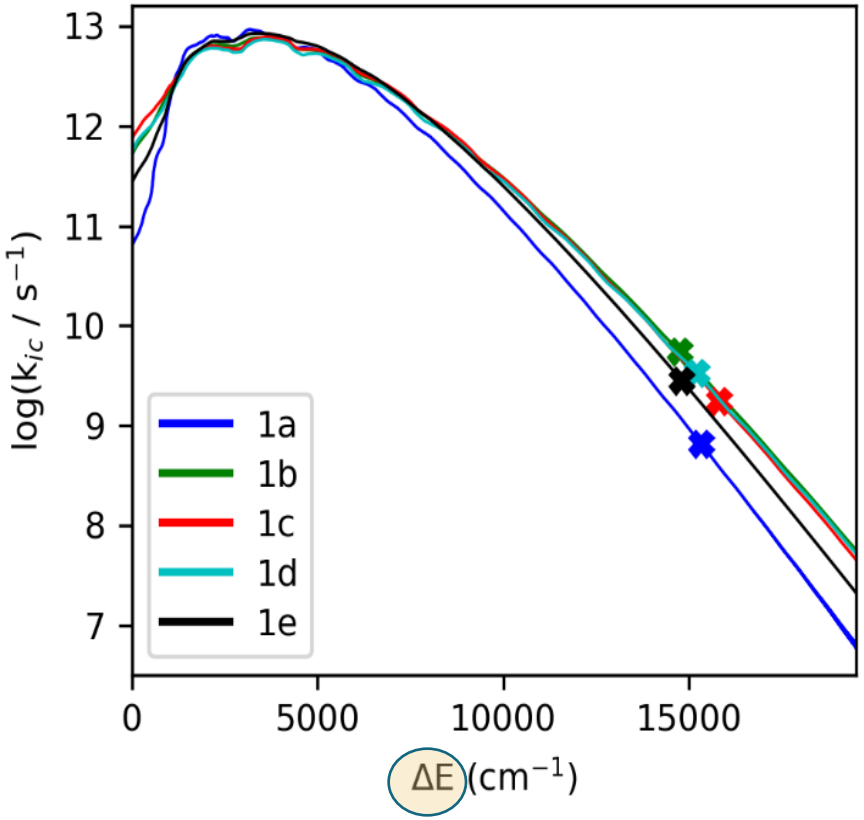
$$FCWD = \frac{1}{\sqrt{4\pi\lambda RT}} \exp\left(-\frac{(\Delta E + \lambda)^2}{4\pi\lambda RT}\right)$$

Small energetic inaccuracies lead to large errors in the k_{IC} rate calculations

K. Veys, D. Escudero, ***J. Phys. Chem A****, 124, 7228 (2020)*

Azulene's anti-Kasha photoluminescence: k_{nr} calculations

- **Translating our TVCF results into a simplified Marcus model:**



$$k_{IC} = \left(\frac{2\pi}{\hbar}\right) H^2 * FCWD$$

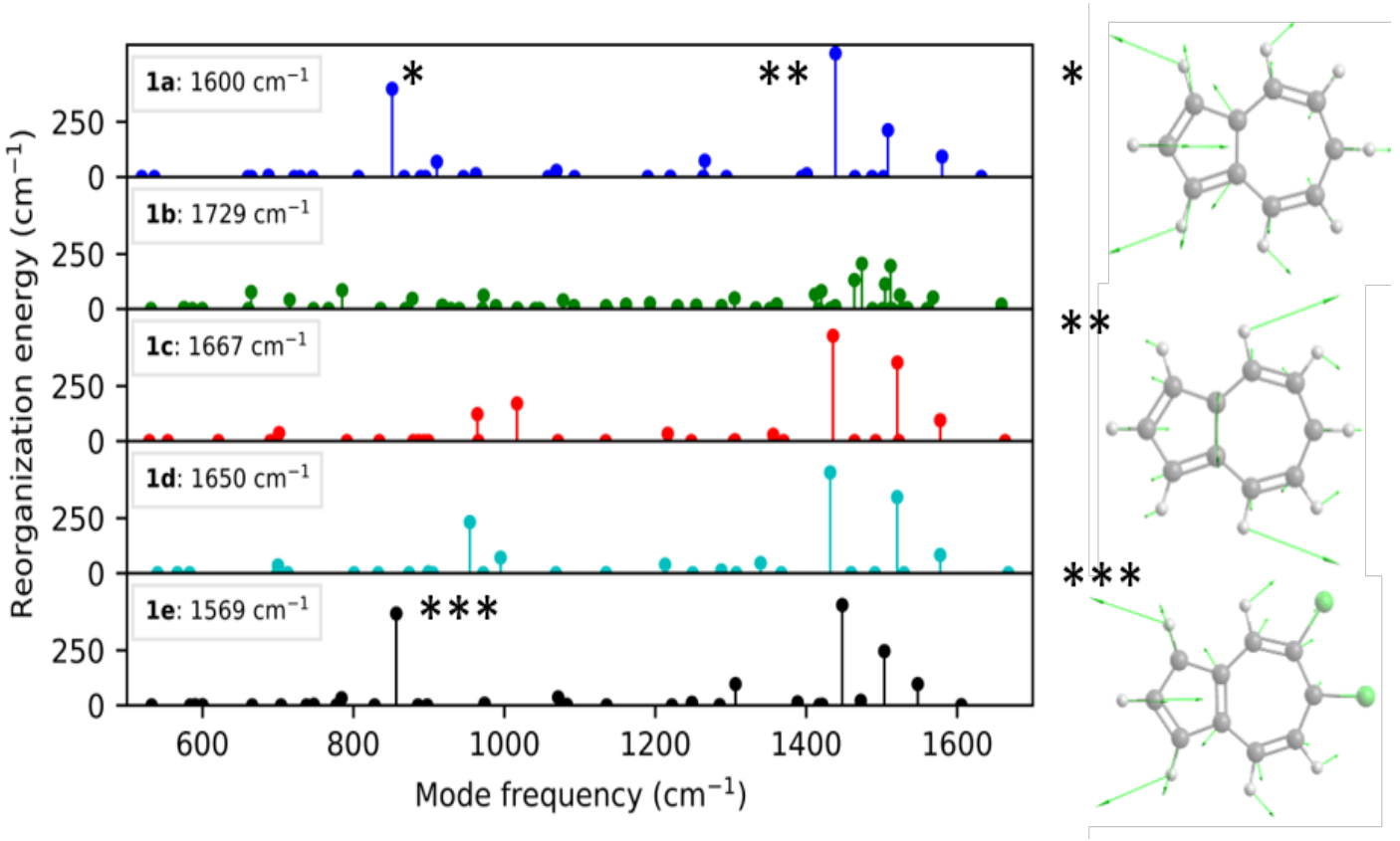
$$FCWD = \frac{1}{\sqrt{4\pi\lambda RT}} \exp\left(-\frac{(\Delta E + \lambda)^2}{4\pi\lambda RT}\right)$$

For **1a-1e**: breakdown of the energy gap law
Reorganization energies (λ) dictate the k_{IC} values

*K. Veys, D. Escudero, **J. Phys. Chem A**, 124, 7228 (2020)*

Azulene's anti-Kasha photoluminescence: k_{nr} calculations

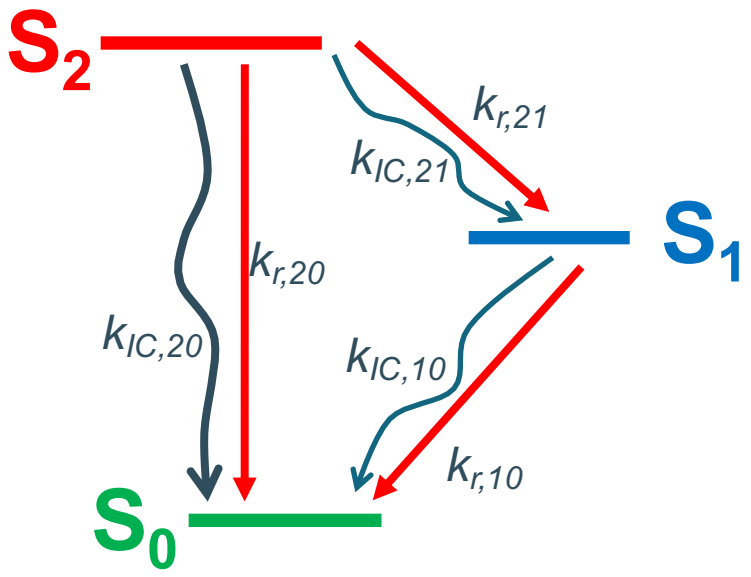
- Reorganization energies (λ) for each mode of **1a-1e:** λ dictate the k_{IC} values:



We can identify the accepting modes promoting the internal conversion decays

K. Veys, D. Escudero, ***J. Phys. Chem A****, 124, 7228 (2020)*

Azulene's anti-Kasha photoluminescence: ϕ_{20} and ϕ_{10}



$$\phi_{20} = k_{r,20} * \tau_2 \approx \frac{k_{r,20}}{k_{r,20} + k_{ic,21}}$$

$$\phi_{10} \approx \frac{k_{r,10}}{k_{r,10} + k_{ic,10}} * \frac{k_{ic,21}}{k_{r,20} + k_{ic,21}}$$

- Computed ϕ_{20} and ϕ_{10} values (experimental values between parentheses):

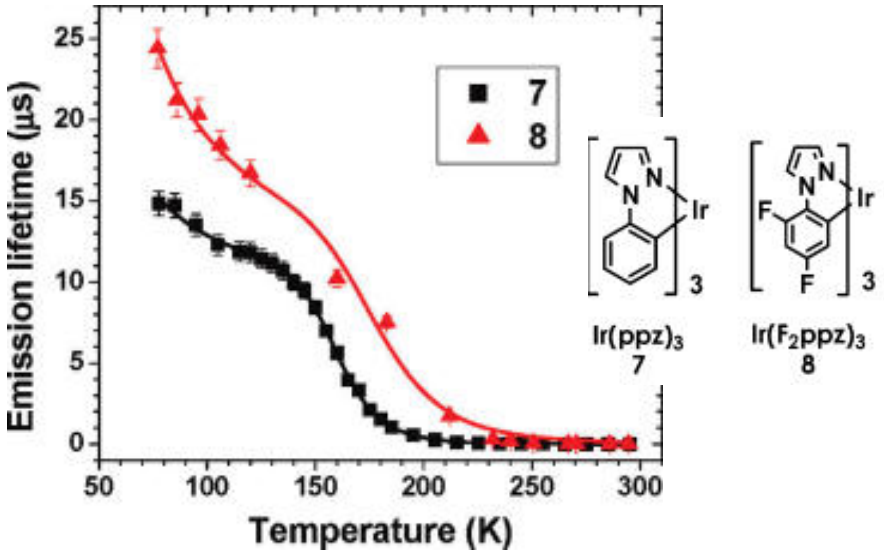
	ϕ (%)	
	$S_1 \rightarrow S_0$	$S_2 \rightarrow S_0$
1a	8.4×10^{-4}	4.3 (3.5±0.4)
1b	1.8×10^{-4}	0.31 (1.5±0.1)
1c	1.9×10^{-4}	1.5 (5.0±0.9)
1d	2.0×10^{-4}	0.82 (1.2)
1e	2.6×10^{-4}	0.44 (2.6)

- Computed and experimental ϕ_{20} and ϕ_{10} values in the same order of magnitude.
- Some of the trends within the series recovered by the calculations.

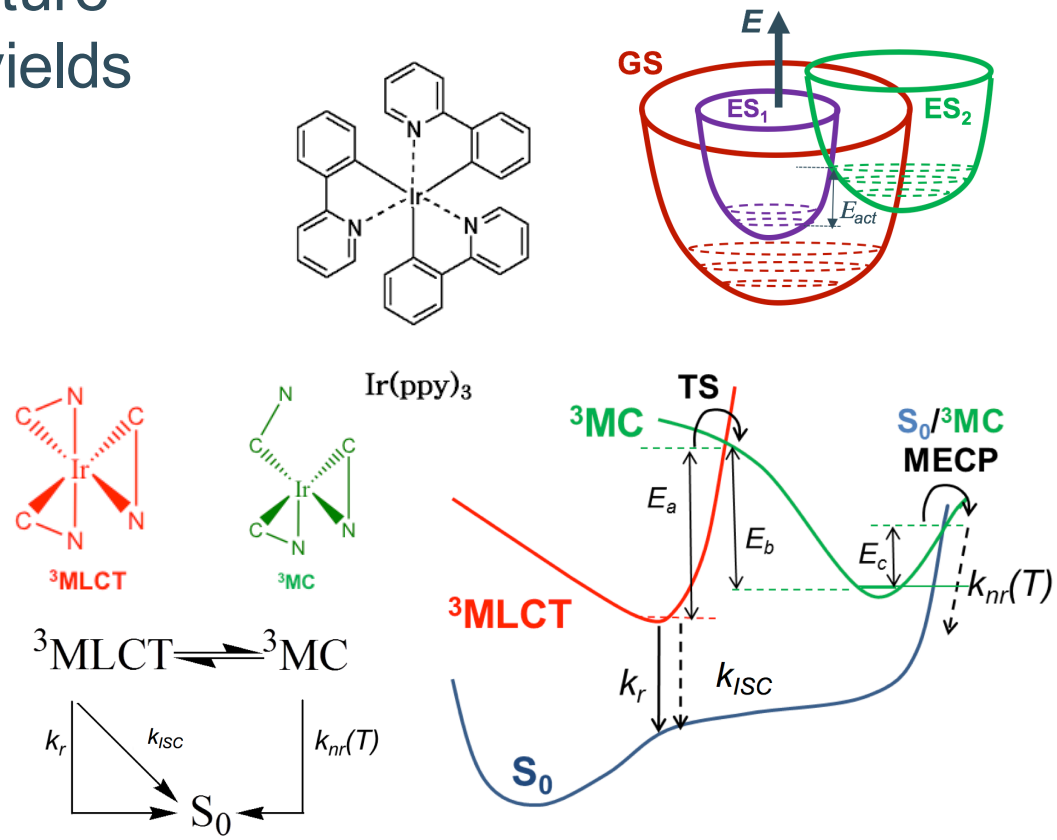
K. Veys, D. Escudero, ***J. Phys. Chem A****, 124, 7228 (2020)*

Outline

- Computational protocol to predict the temperature-dependent photoluminescence lifetimes and yields of phosphors.



Thompson et. al. *J. Am. Chem. Soc.*, **2009**, 131, 9813.



D. Escudero, et. al. *Chem. Eur. J.* **2013**, 19, 15639

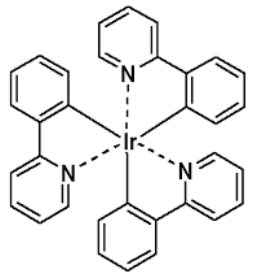
Excited-state modelling of phosphors

- For phosphor molecules: **Ir(III), Re(I), Ru(II), Pt(II) ccomplexes:**

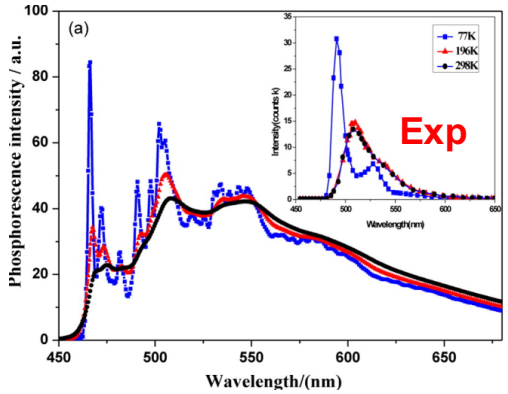
TD-DFT errors: 0.1-0.4 eV:
Hybrid xc functionals with 20-25% HF exchange outperform the rest of functionals for vertical excitation energies. Balanced description of all possible excited states: MC, MLCT, LC, etc.

D. Escudero, L. González. JCTC, 8, 203 **(2012)**
D. Escudero, W. Thiel. JCP, 140, 194105 **(2014)**
L. Freitag, L. González et al. *Coord. Chem. Rev*. 304, 146 **(2015)**
C. Daniel, Top. Curr. Chem. **368**, 377-413 **(2016)**
F. Plasser et al., *J. Phys. Chem. A*, **119**, 1023 **(2015)**

- **Prediction of color:** Accurate computed emission energies + vibronic couplings.



$Ir(ppy)_3$



Q. Peng, Z. Shuai et al., *J. Chem. Theory and Comput.*, **9**, 1132 **(2013)**

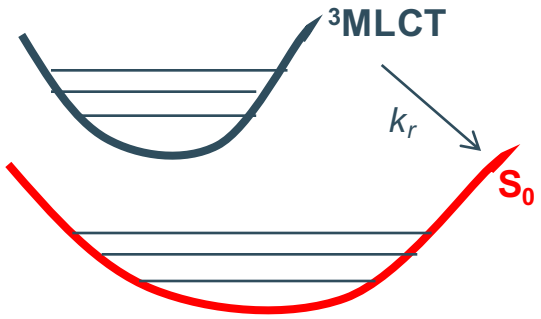
- **Can we predict the phosphorescent lifetimes and efficiencies?**

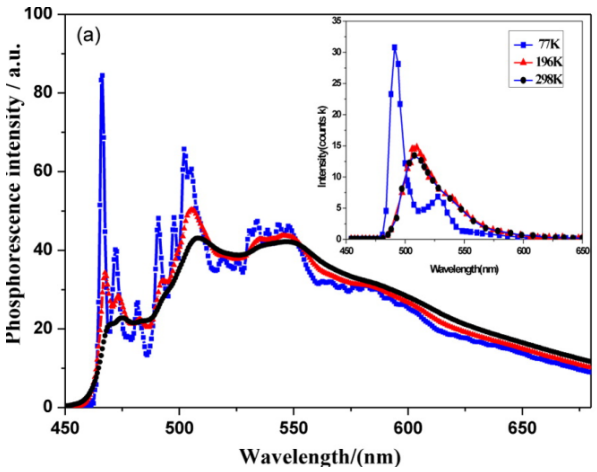
- $\Phi_{phos} = k_r / (k_r + \sum k_{nr})$
- $\tau = 1 / (k_r + \sum k_{nr})$

- k_r easy to compute provided that only 1 state is involved in emission
- $\sum k_{nr}$ are cumbersome to compute

Excited state decay rate theory: calculation of k_r

❑ k_r : Einstein spontaneous emission





$$k_r^i = k_r(S_0, T_{em}^i) = \frac{4\alpha_0^3}{3t_0}\Delta E_{S-T}{}^3 \sum_{j\in\{x,y,z\}} \left|M_j^i\right|^2$$

$$M_j^i = \sum_{n=0}^{\infty} \frac{\langle S_0|\hat{\mu}_j|S_n\rangle\langle S_n|\hat{H}_{SO}|T_{em}^i\rangle}{E(S_n)-E(T_{em})} + \sum_{n=0}^{\infty} \frac{\langle S_0|\hat{H}_{SO}|T_n\rangle\langle T_n|\hat{\mu}_j|T_{em}^i\rangle}{E(T_n)-E(S_0)}, j \in \{x,y,z\}$$

- Self-consistent SOC-TDDFT (ADF)
- Perturbative SOC-TDDFT (ADF, BDF)
- QR-TDDFT (Dalton)

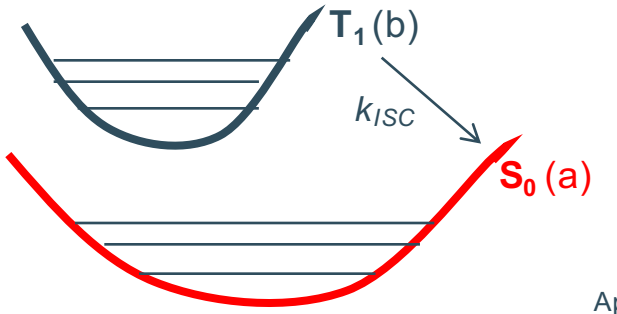
❖ Are the k_r values temperature dependent?

$$k_r = \frac{k_{r,I} + k_{r,II}exp(-E_{II,I}/k_BT) + k_{r,III}exp(-E_{III,I}/k_BT)}{1 + exp(-E_{II,I}/k_BT) + exp(-E_{III,I}/k_BT)}$$

YES! Boltzmann distribution of the three spin sublevels

Excited state decay rate theory: calculation of k_{nr} (k_{ISC})

- k_{nr} (i.e., k_{ISC}) is computed with **Thermal Vibration Correlation Function** (TVCF)[1] theory.



$$k_{b\to a} = \frac{2\pi}{\hbar}\sum_{vu} P_{av}\left|H'_{bu,av} + \sum_{cw}\frac{H'_{bu,cw}H'_{cw,av}}{E_{bv}-E_{cw}}\right|^2 \delta(E_{av}-E_{bu})$$

where $H'\Psi_{av} = -\hbar^2\frac{\partial\Phi_a}{\partial Q_{bl}}\frac{\partial\Theta_{av}}{\partial Q_{bl}} + H^{SO}\Phi_a\Theta_{av}$

Applying TVCF and Condon Approximations:

$$k_{isc}^{(0)} = \frac{1}{\hbar^2}R_{ba}^{isc}\int_{-\infty}^{\infty} dt e^{i\omega_{ab}t}\rho_{isc}^{(0)}(t,T)$$

[1] Z. Shuai et. al., *J. Chem. Theory and Comput*, **9**, 1132 (**2013**)

- Multidimensional harmonic oscillator model coupled to DFT and TD-DFT calculations where displacements, distortions and Duschinsky rotations of the PES (**MOMAP**)[2]

We need: GS and ES geometries, 2nd derivatives, SOCs, etc.

[2] Shuai, Z.; Peng, Q.; Niu, Y. L.; Geng, H. MOMAP, a Free and Open-Source Molecular Materials Property Prediction Package, revision 0.2.004; Shuai group: Beijing, CN, 2014, http://www.shuaigroup.net/

Excited state decay rate theory: calculation of $k_{nr}(T)$

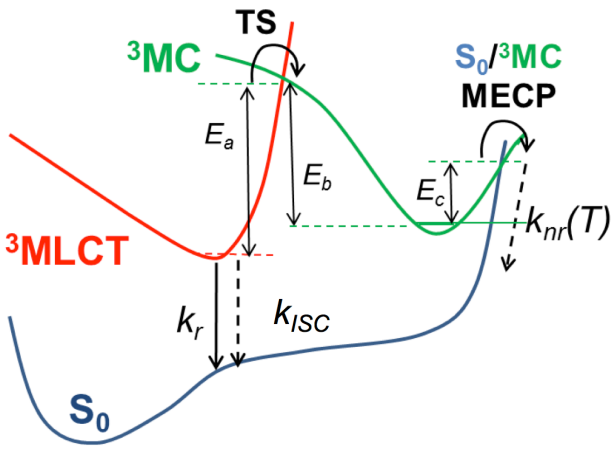
- k_{nr}(T) :

$$^3\text{MLCT} \underset{k_b}{\overset{k_a}{\rightleftharpoons}} {}^3\text{MC} \xrightarrow{k_c} S_0$$

$$d(^3\text{MC})/dt = 0 \longrightarrow k_{nr}(T) = k_c k_a/(k_c + k_b)$$

$$E_a > E_b > E_c : \quad k_{nr}(T) = A_0 A \exp(-E_a/k_B T),$$

$$\text{where} \quad A_0 = \frac{1}{1 + \exp\left(\frac{E_c - E_b}{k_B T}\right)}$$



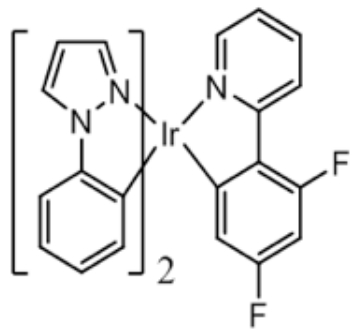
- Prefactor (A) obtained with **canonical variational transition state** (CVT) dynamics, based on the computed UDFT energy profiles for the thermally activated nonradiative decay (**POLYRATE**)[3]

We need: Accurate E_a values (PWPB95-D3/6-31G*)[4] and the IRC profiles

[3] *Zheng, J. et al. POLYRATE, version 2010; University of Minnesota: Minneapolis, MN, 2010*

[4] Steinmetz, M et. al. *ChemistryOpen* **2013**, *2*, 115

Blue Phosphor

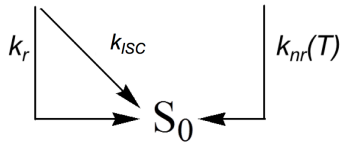


fac-$(F_2ppz)_2Ir(ppy)$ (**3**)

$$\tau(T) = \frac{1}{k_r + k_{ISC} + k_{nr}(T)} \qquad \Phi_P(T) = \frac{k_r}{k_r + k_{ISC} + k_{nr}(T)}$$

Temperature (K)	k_r (s^{-1})	k_{ISC} (s^{-1})	k_{nr} (T) (s^{-1})	Global Lifetime (μs)	Φ_P
77	1.5994×10^4	1.7781×10^5	4.433E-12	5.1598	0.083
196	1.8236×10^5	2.9713×10^5	4.933E+03	2.0405	0.384
298	3.0281×10^5	6.0007×10^5	5.691E+06	0.1516	0.046
400	3.8287×10^5	1.4561×10^6	2.166E+08	0.0046	0.002

^{3}MLCT $\rightleftharpoons$ ^{3}MC



$$k_r = \frac{k_{r,I} + k_{r,II}exp(-E_{II,I}/k_BT) + k_{r,III}exp(-E_{III,I}/k_BT)}{1 + exp(-E_{II,I}/k_BT) + exp(-E_{III,I}/k_BT)}$$

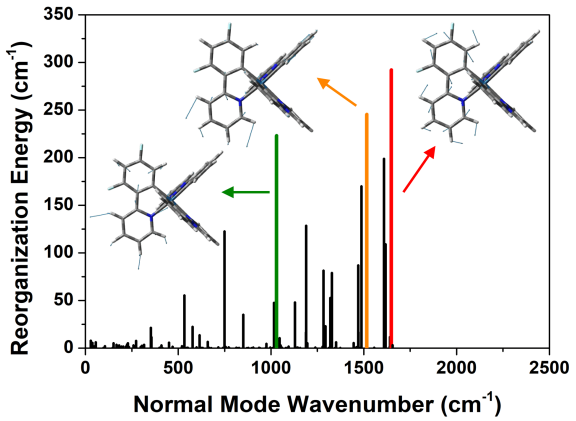
CVT dynamics:

$$k_{nr}(T) = AA_0\exp(-E_a/k_BT)$$

A (s^{-1}) = 1.47×10^{13}

E_{act} = 2836 cm^{-1} (PWPB95-D3/6-31G*)

❑ k_{ISC} :



$$\ln\left[k_{nr}(T_1 \rightarrow S_0)\right] = -\frac{\left(\Delta E_{ad} - \sum_k \lambda_k\right)^2}{4\sum_k \lambda_k \bar{E}_k} + \ln\left(\frac{1}{\hbar}\left|\left\langle S_0\left|\hat{H}^{SO}\right|T_1\right\rangle\right|^2 \sqrt{\frac{\pi}{\sum_k \lambda_k \bar{E}_k}}\right)$$

Computational details:

k_r / k_{nr} / SOCs: TD-B3LYP/6-31G(d,p)/LANL2DZ

k_{nr} (T): PWPB95-D3/6-31G*// B3LYP/6-31G-d,p)

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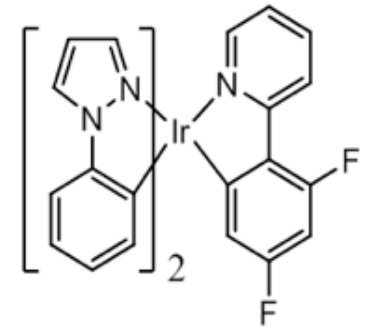
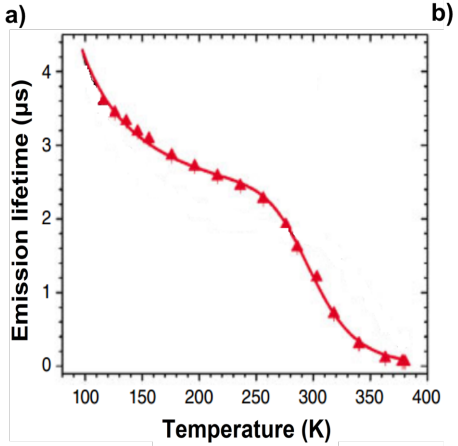
Blue Phosphor



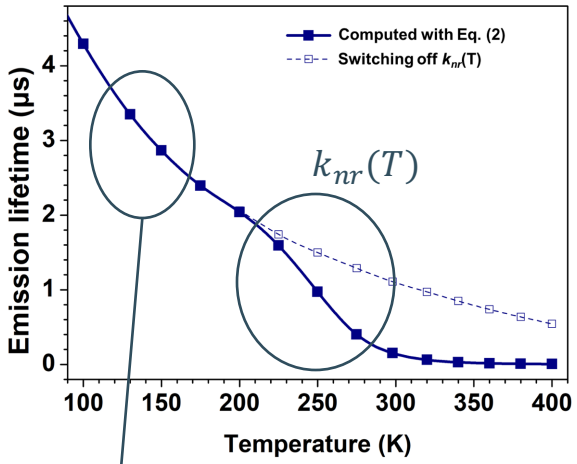
fac-$(F_2ppz)_2Ir(ppy)$ (**3**)

Experimental



Thompson et. al. *J. Am. Chem. Soc.*, **2009**, 131, 9813.

Computed



$$k_r = \frac{k_{r,I} + k_{r,II}exp(-E_{II,I}/k_BT) + k_{r,III}exp(-E_{III,I}/k_BT)}{1 + exp(-E_{II,I}/k_BT) + exp(-E_{III,I}/k_BT)}$$

- **Phosphorescent efficiencies** and lifetimes can be estimated at any given temperature.

Φ (theo, RT)	Φ (theo, 196K)
0.05	0.39

- **This protocol** can be applied to **all-kind of Ir(III) complexes** (from blue to red)
- Can be used for the automatic in silico prescreening of phosphors for PhOLEDs

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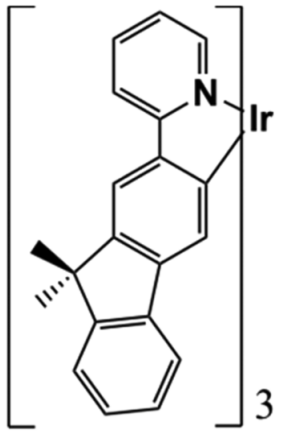
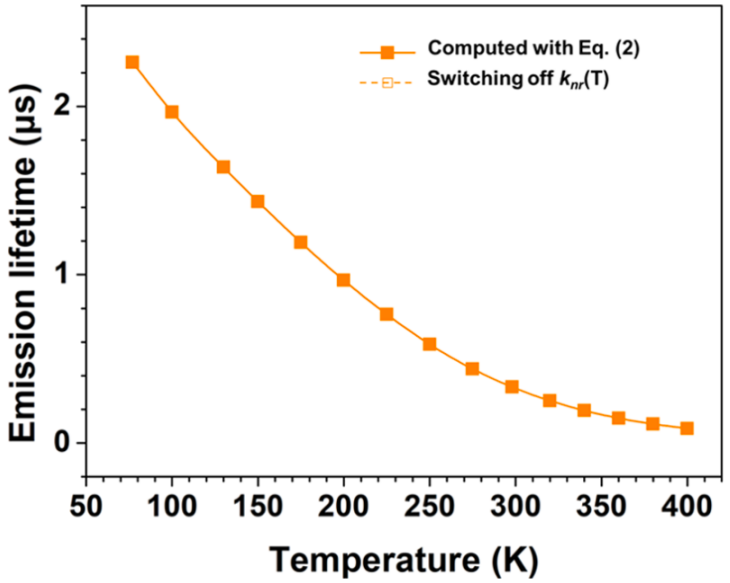
Yellow/Orange Phosphor



fac-Ir(flpy)$_3$

$$\tau(T) = \frac{1}{k_r + k_{ISC} + k_{nr}(T)} \qquad \Phi_P(T) = \frac{k_r}{k_r + k_{ISC} + k_{nr}(T)}$$

Temperature(K)	k_r (s^{-1})	k_{ISC} (s^{-1})	k_{nr} (T) (s^{-1})	Global Lifetime (μs)	Φ_P	
77	1.9351×10^5	2.4871×10^5	2.201E-33	2.2613	0.438	
200	2.4398×10^5	7.9016×10^5	3.551E-05	0.9670	0.236	
298	2.5399×10^5	2.7525×10^6	2.243E+01	0.3326	0.084	**Exp=0.29**



CVT dynamics:

$A\ (s^{-1}) = 1.97\times10^{13}$

E_{act} = 5182 cm^{-1} (PWPB95-D3/6-31G*)

DESIGN RULE to attain large Φ_P values at RT: E_{act} > 4000 cm^{-1}

Computational details:

k_r / k_{nr} / SOCs: TD-B3LYP/6-31G(d,p)/LANL2DZ

k_{nr}(T): PWPB95-D3/6-31G*// B3LYP/6-31G-d,p)

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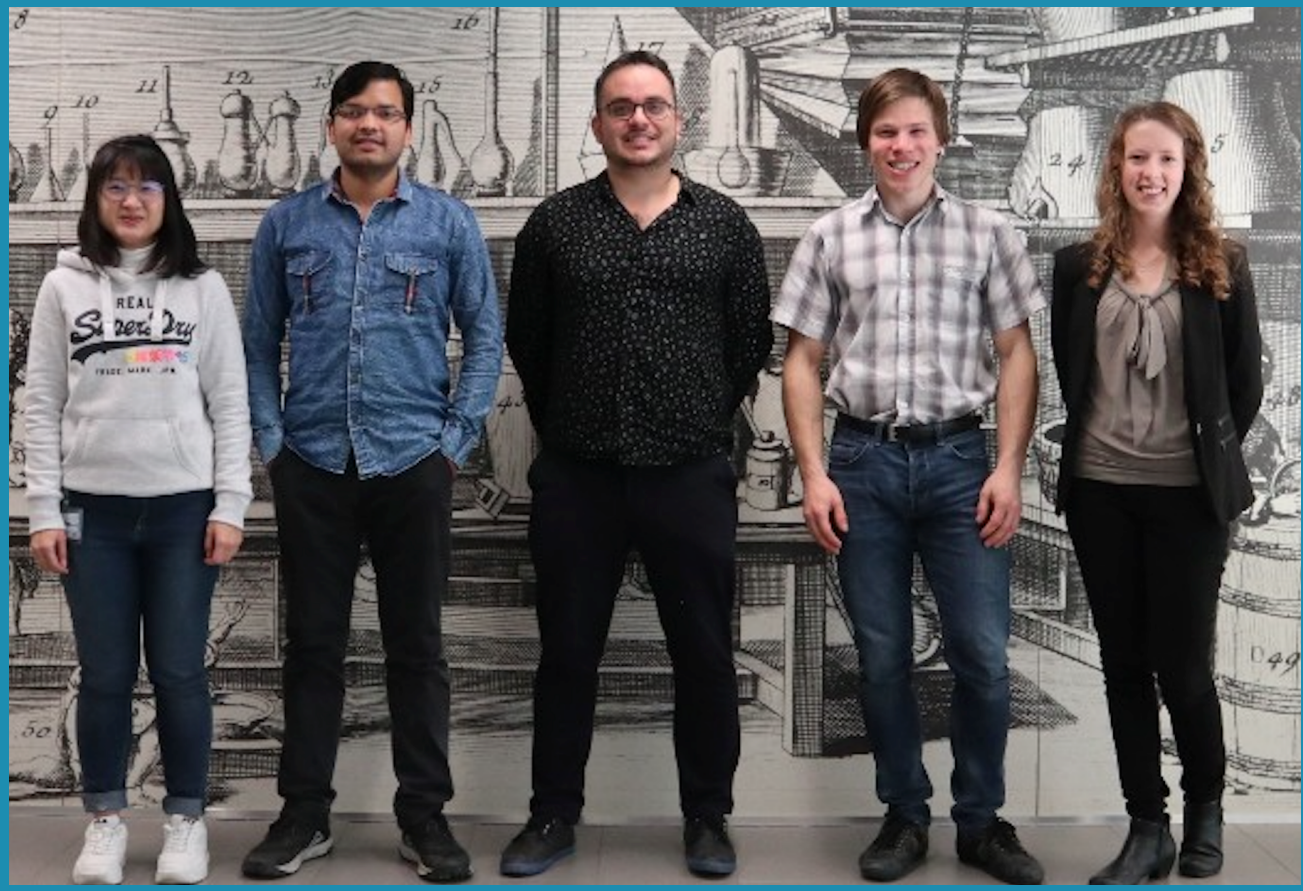
Sylvio Arroliga-Rocha
Marziogiuseppe Gentile

PhD students:
Koen Veys
Prashant Kumar



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