Transfers leading to scintillation

D. González-Díaz (IGFAE)
on behalf of the Pyboltz team

talk prepared for the topical workshop 'new horizons in TPCs'
(Santiago de Compostela, 05-10-2020)

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Electron transport in gaseous detectors with a Python-based Monte Carlo simulation code☆

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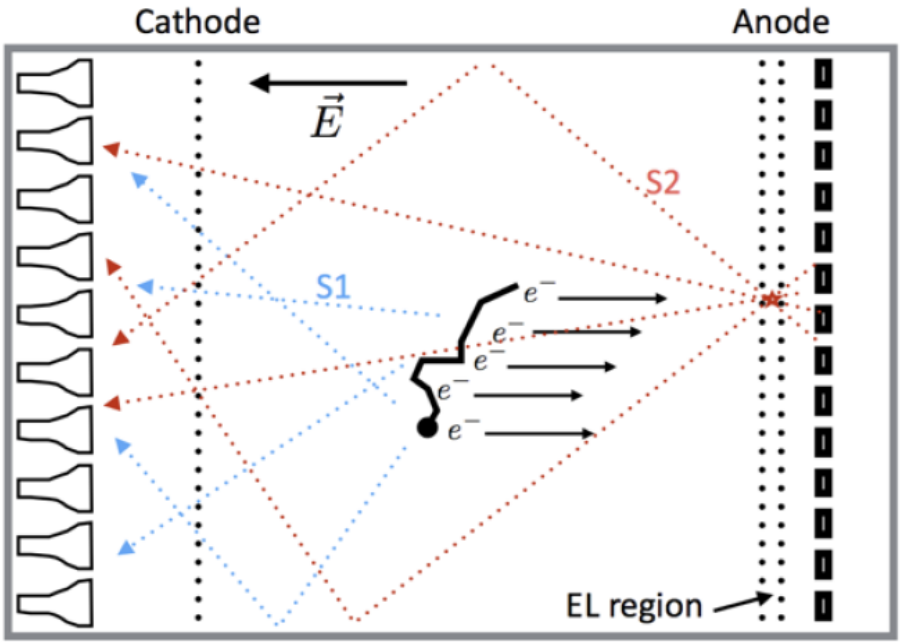
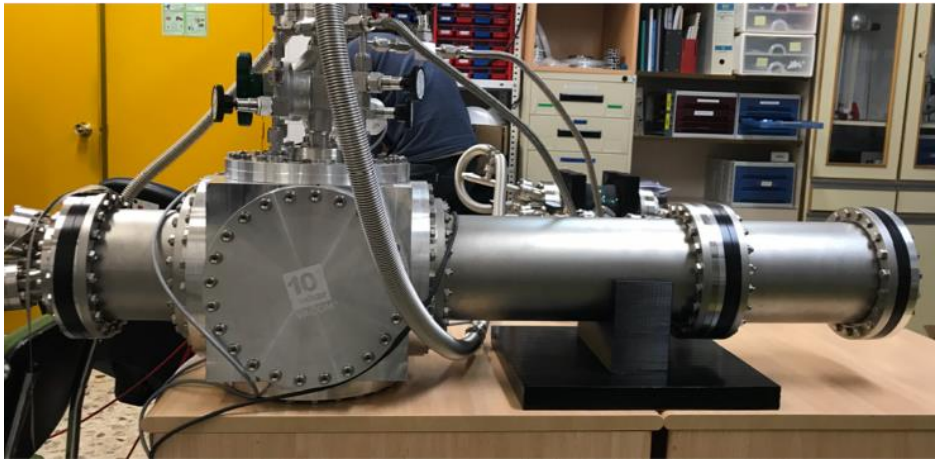
scintillation-based TPCs (why?)

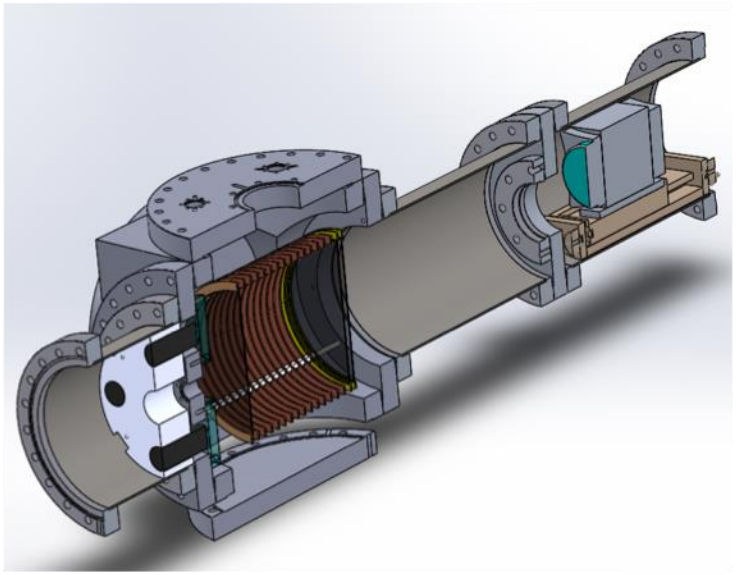
- **Lower energy threshold** in noble element TPCs, potentially down to ~20eV (XENON/LZ/PANDA-X, DarkSide, ARIADNE).
- **To/S1 information** for volume fiducializacion, spill-assignment, particle ID (NEXT, DUNE TPCs, ARIADNE, XENON/LZ/PANDA-X, DarkSide).
- **Higher resolution images** (DMTPC, CYGNO, ARIADNE, Migdal-TPC, IGFAE fission-TPC).
- **Energy resolution close to Fano Factor, if using electroluminescence** (NEXT).
- **Low, potentially zero, ion feedback,** suppresses space-charge issues in the drift region (ARIADNE).

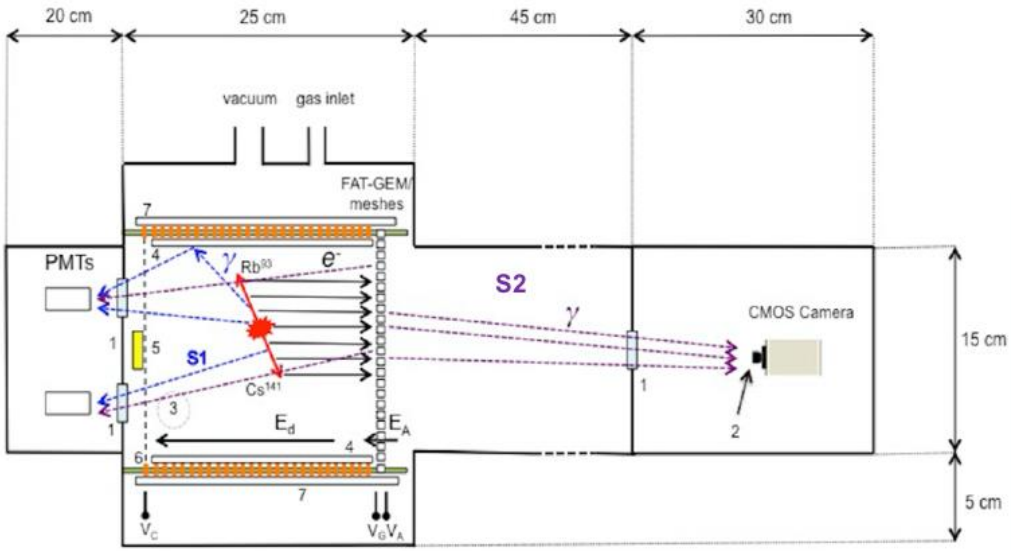
- Higher immunity to electrical noise, and discharges. In some cases, less complexity and affordability.

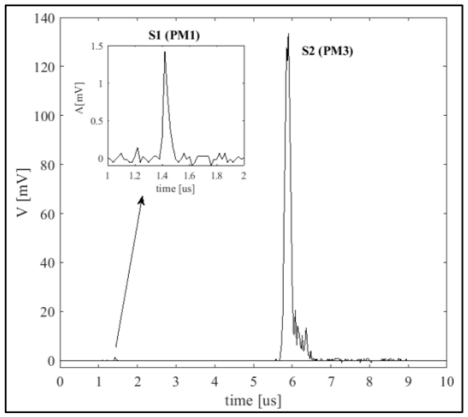


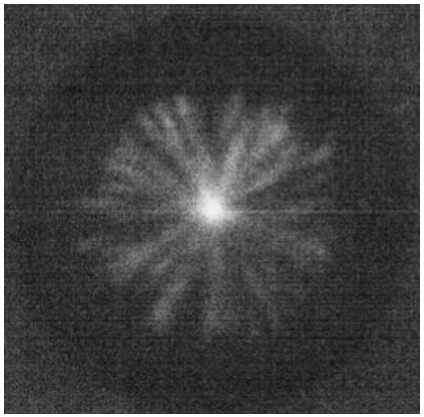
IGFAE fission-TPC (technology demonstrator)





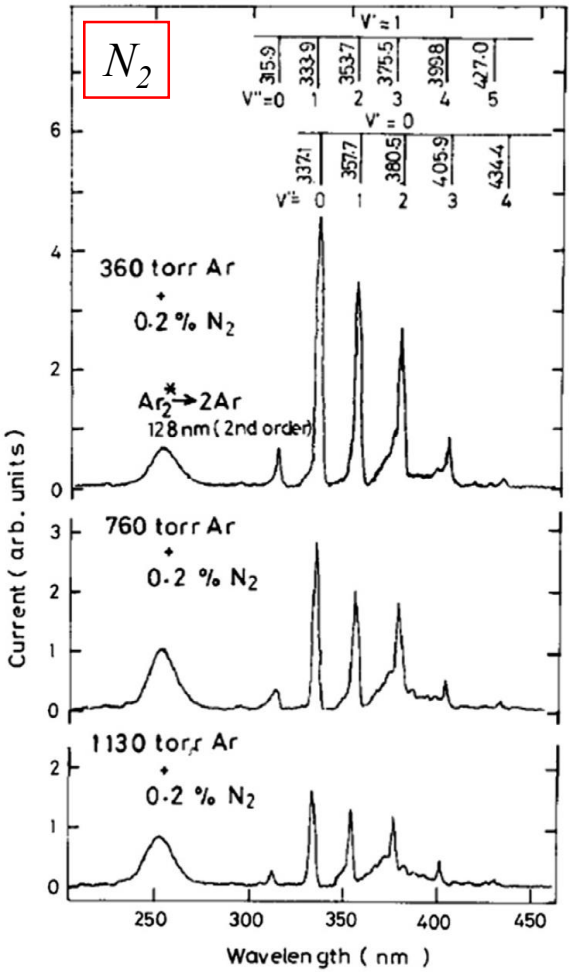


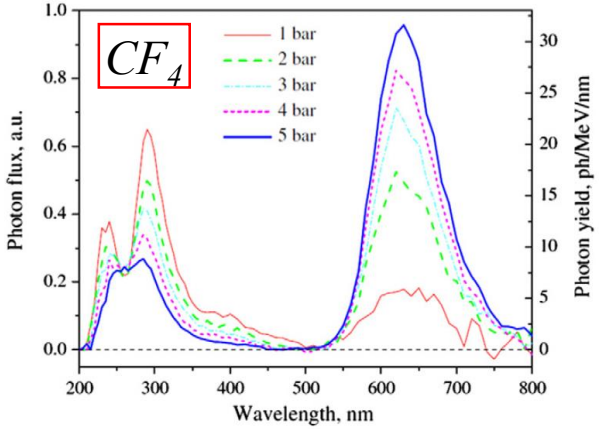


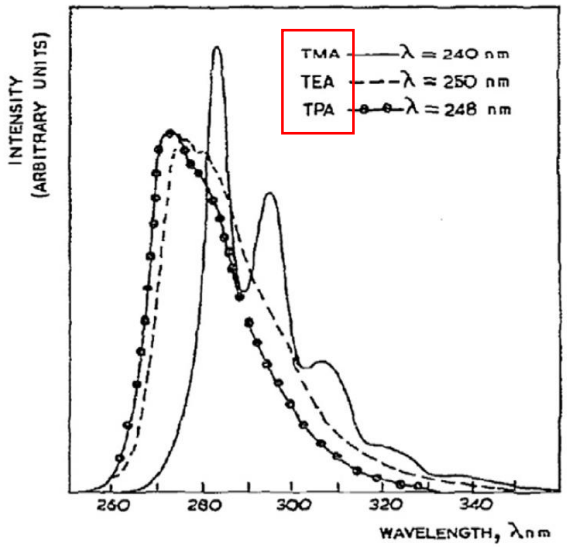


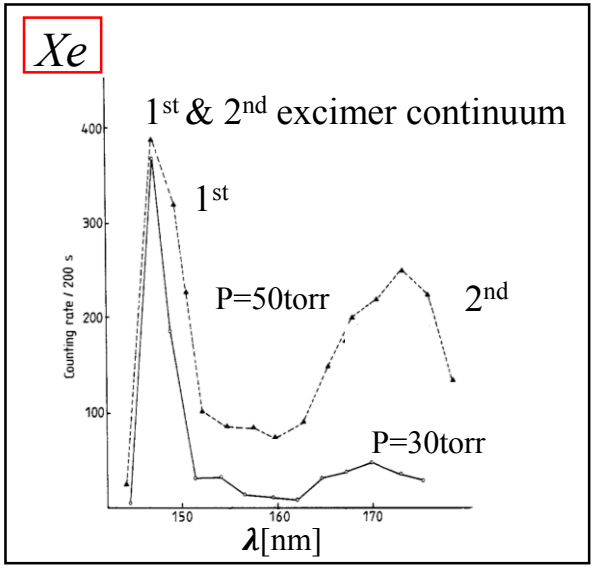
reconstruction of alpha particles in CF_4 (0.5bar)

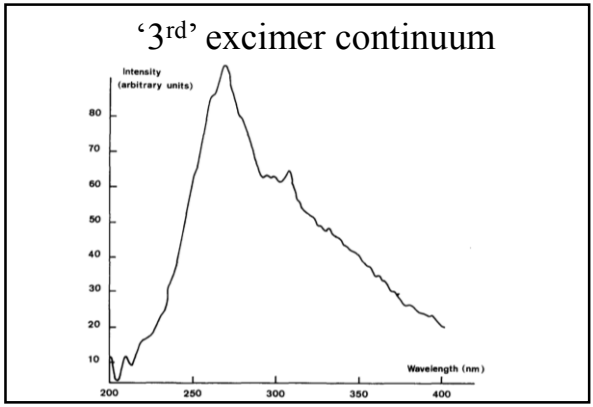
scintillation in familiar gases

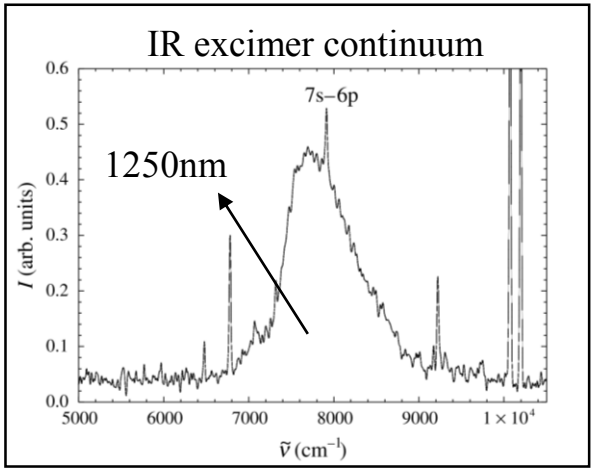












and…

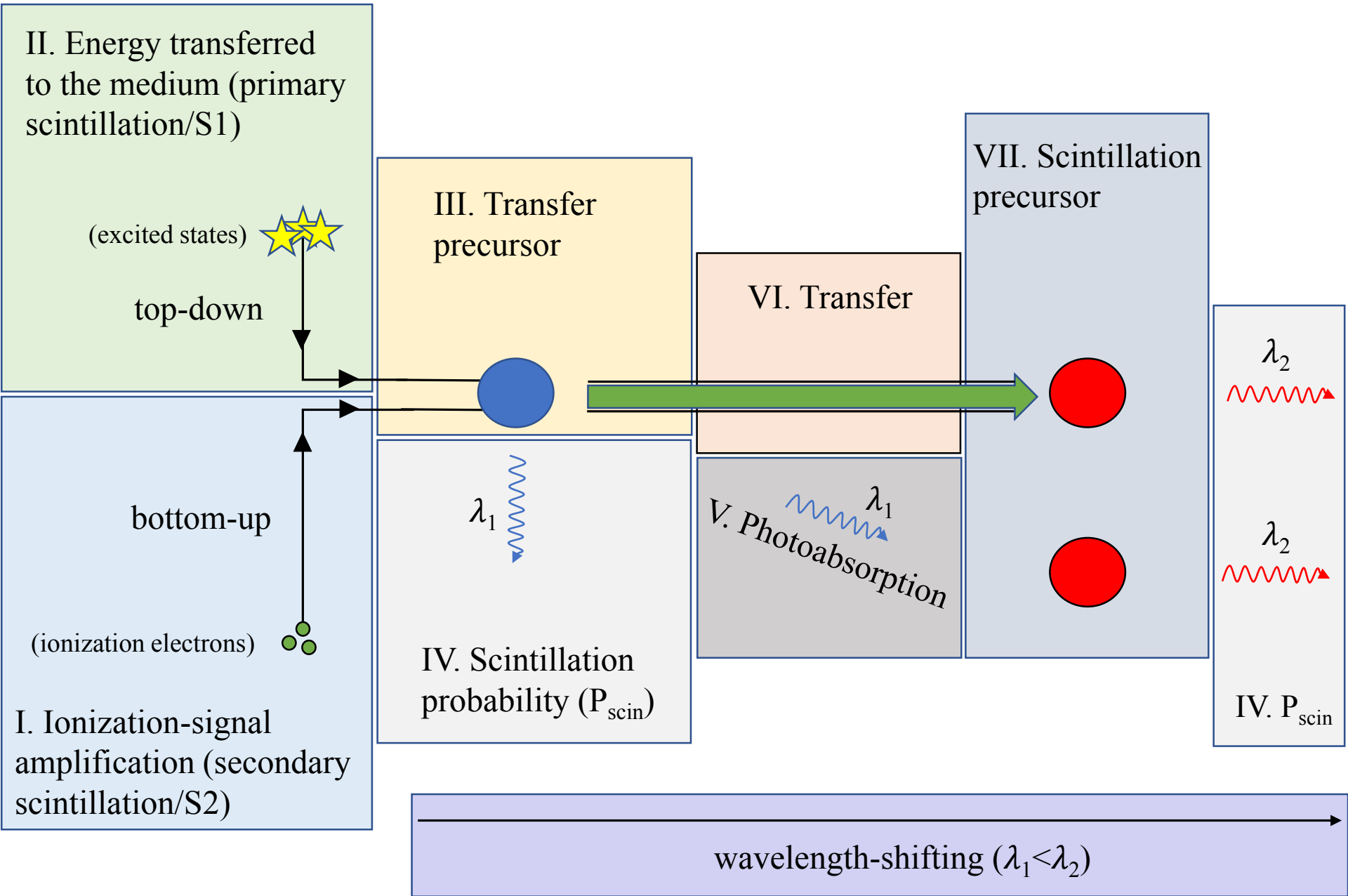
molecular electroluminescence (CF_4) [E. Baracchini et al. JINST 15(2020)]

neutral/polarization bremsstrahlung in argon [A. Buzulutskov et al. Astropart. Phys 103(2018)29]

neutral/polarization bremsstrahlung in xenon [C. Henriques, P. Amedo et al, at this workshop]

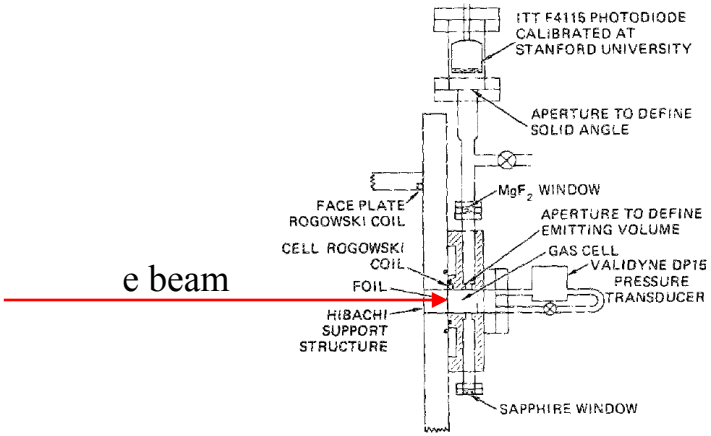
…

how scintillation operates at 'high' pressures (>100mbar)



modelling these type of situations is relatively common

D.C. Lorents, Physica 82C (1976) 19.
D.J. Eckstrom, J. Appl. Phys. 64 (1988) 1679.
Thomas H. Johnson, et al., J. Appl. Phys. 66 (1989) 5707.



excimer laser

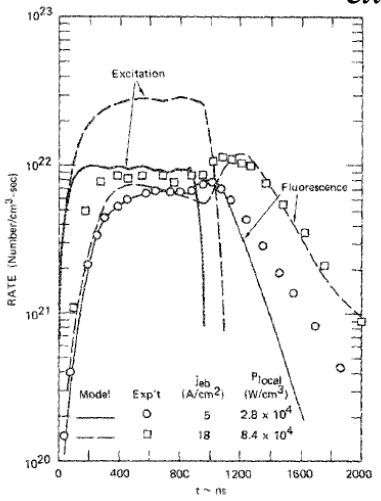


FIG. 3. Excitation rate and excimer fluorescence rate histories for *e*-beam-pumped xenon at 0.5 atm. Excitation rates apply to both the experiments and the model.

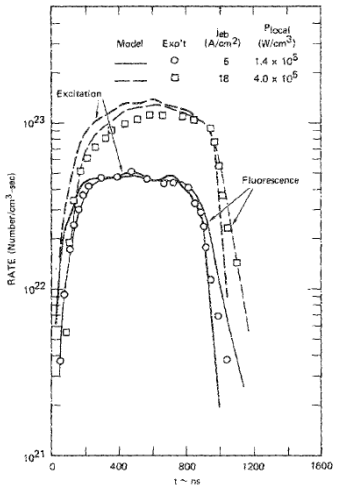
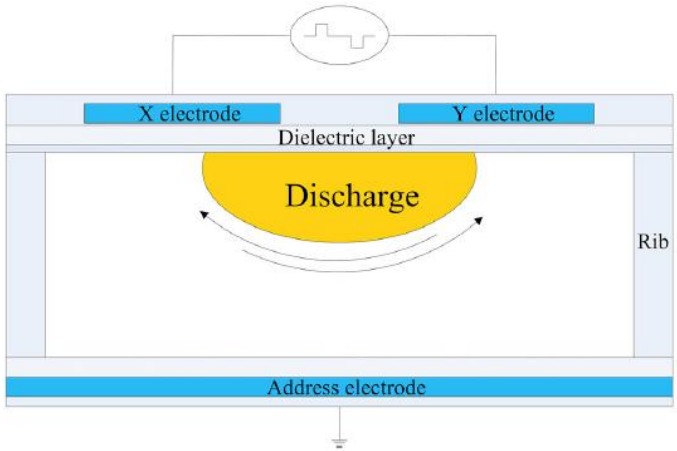
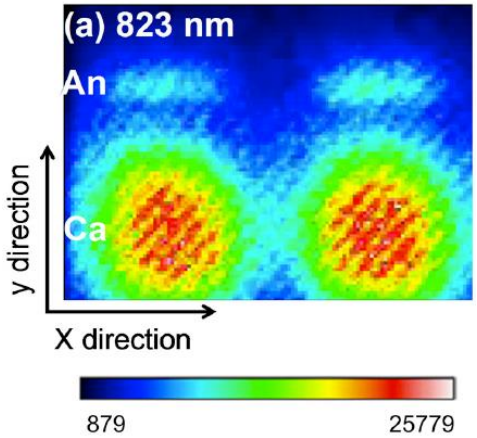


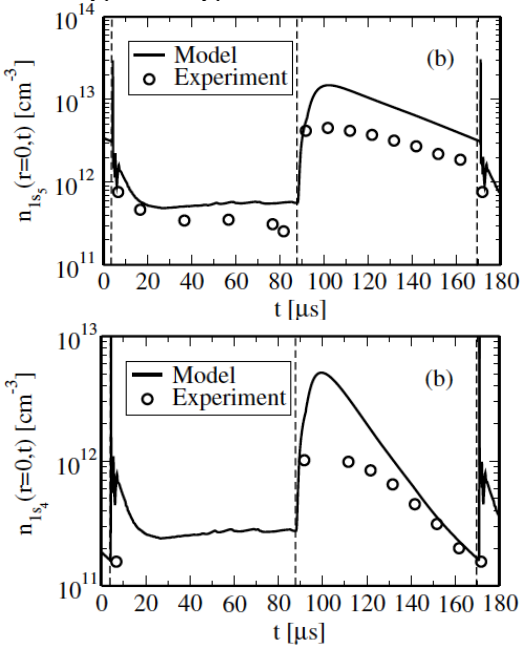
FIG. 5. Excitation rate and excimer fluorescence rate histories for *e*-beam-pumped xenon at 3 atm.

discharges in gases

M. Gnybida, D. Uhrlandt, D. Loffhagen, J. Phys. D 45 (2012) 195203.
Di. Zhu, Xiong Zhang, Hiroshi Kajiyama, J. Appl. Phys. 112 (2012) 033304.

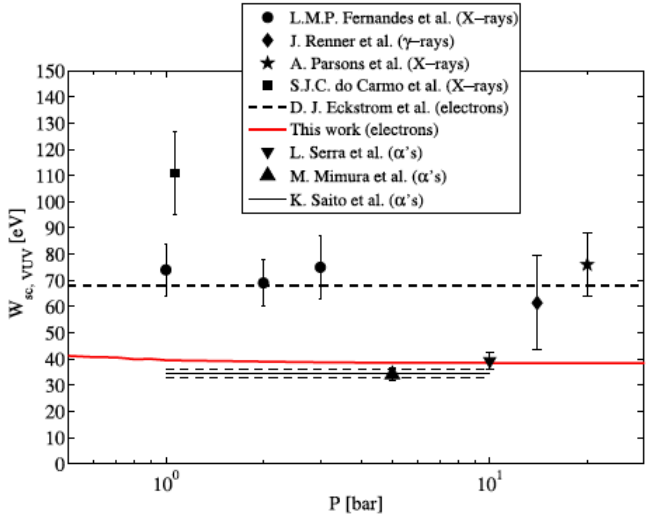






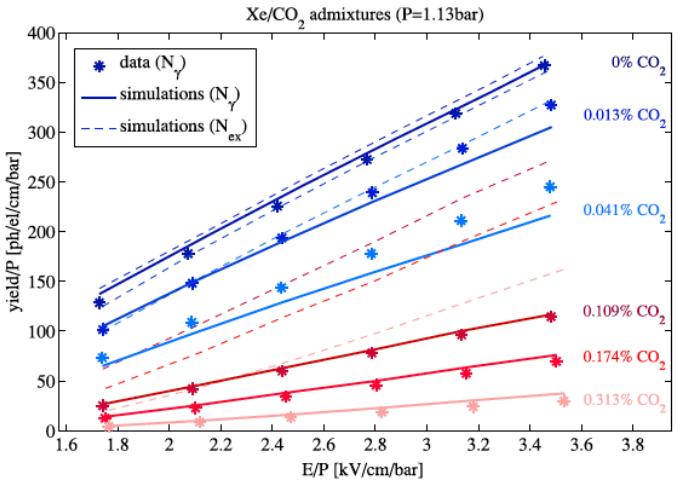
…and it can be done in conditions of interest to gaseous detectors, too!

primary scintillation



wavelength spectrum

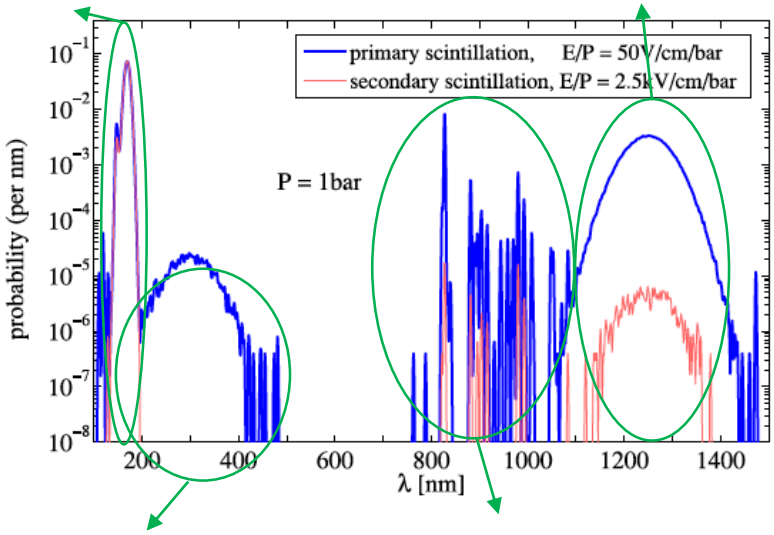
secondary scintillation



time spectrum

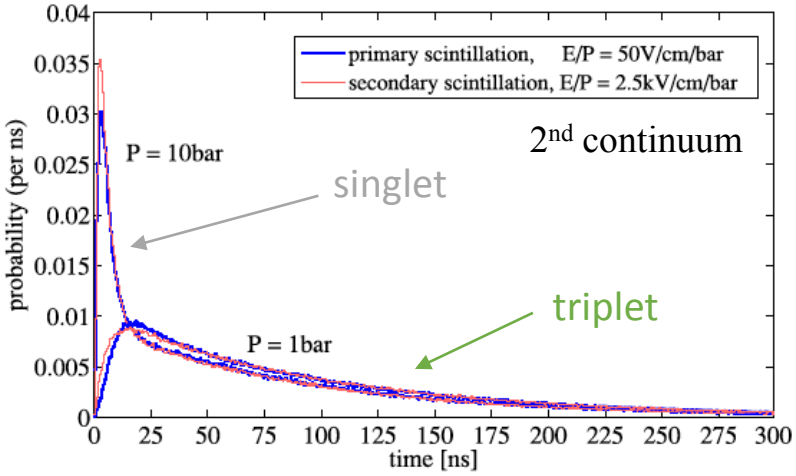
1st & 2nd excimer continuum

IR excimer continuum



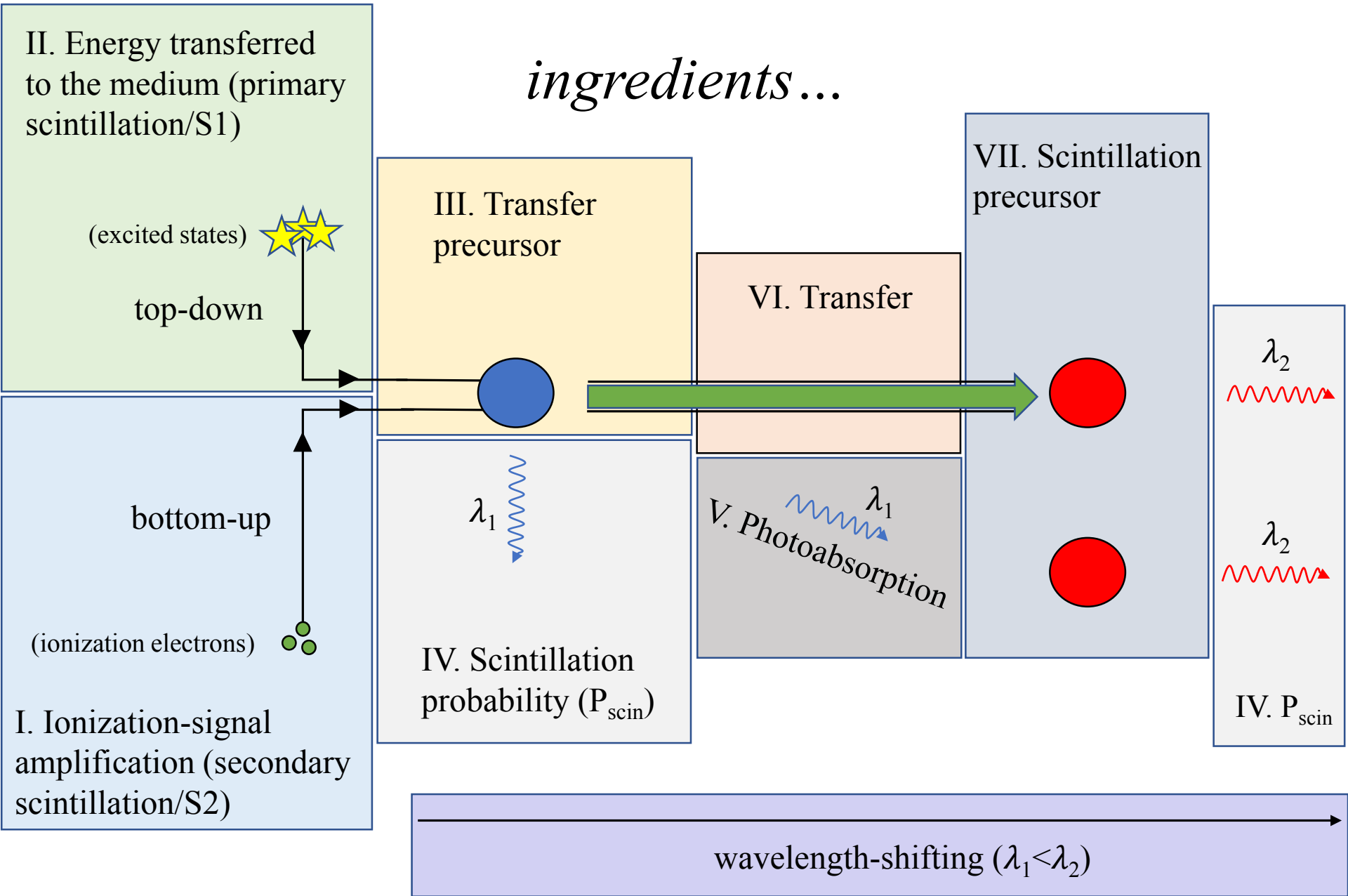
'3rd' excimer continuum

atomic lines

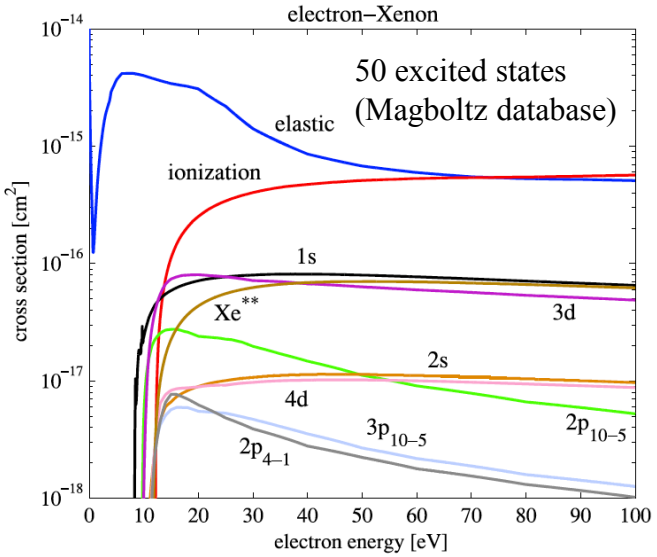


C. Azevedo, D. Gonzalez-Diaz, et al., Microscopic simulation of xenon-based optical TPCs in the presence of molecular additives, Nucl. Instrum. Methods. Phys. Res. A 877 (2018) 157.

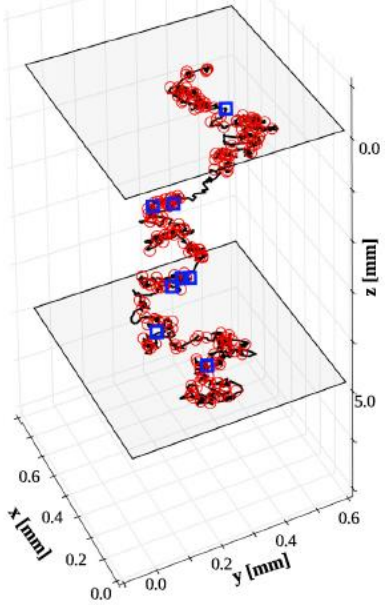
how scintillation operates at 'high' pressures (>100mbar)



Magboltz/Pyboltz allows performing this calculation



1 ionization electron in 5mm gap (E=2.5kV/cm/bar)



○ Low-lying states

□ High-lying states

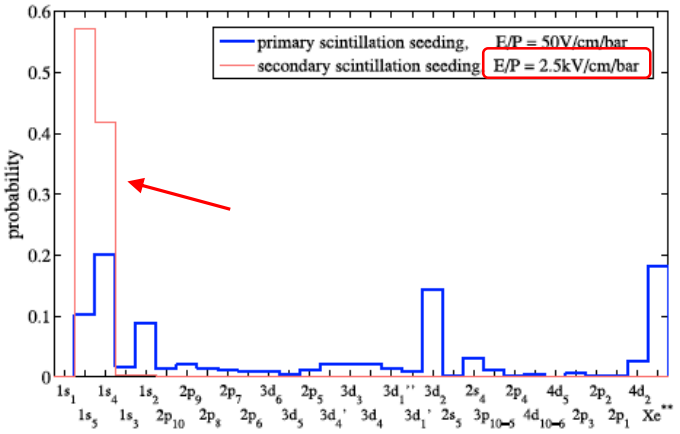
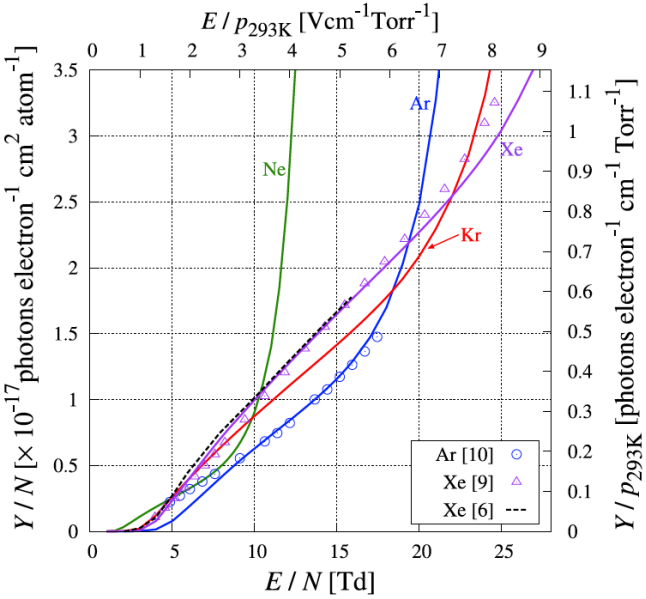


Fig. 1. Simulated probability distributions for the first 41 excited states of xenon upon interaction of a 30 keV electron. The primary scintillation seeding (thick lines) refers to the case where the excited states are directly promoted by the impinging electron; in the secondary scintillation case the seeding is generated by the ionization electrons, with assistance from an external field at a convenient location (thin lines).

bottom-up

(ionization electrons)

I. Ionization-signal amplification (secondary scintillation/S2)



assume pure gas:
1 excited state = 1 VUV photon

C. A. O. Oliveira, H. Schindler, R. J.Veenhof, S. Biagi et al
Phys. Lett. B 703(2011)217

Degrad allows detailed computation of seed states for S1 (works for electrons, mips and x-rays)

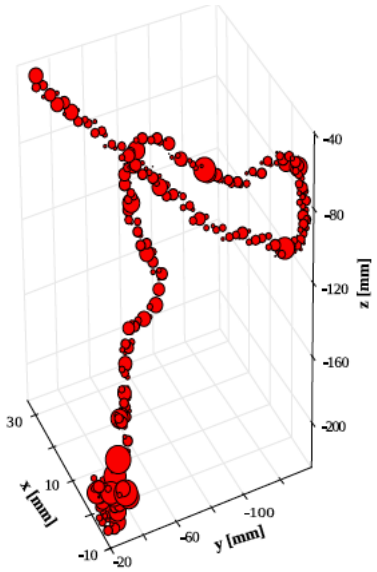
II. Energy transferred to the medium (primary scintillation/S1)

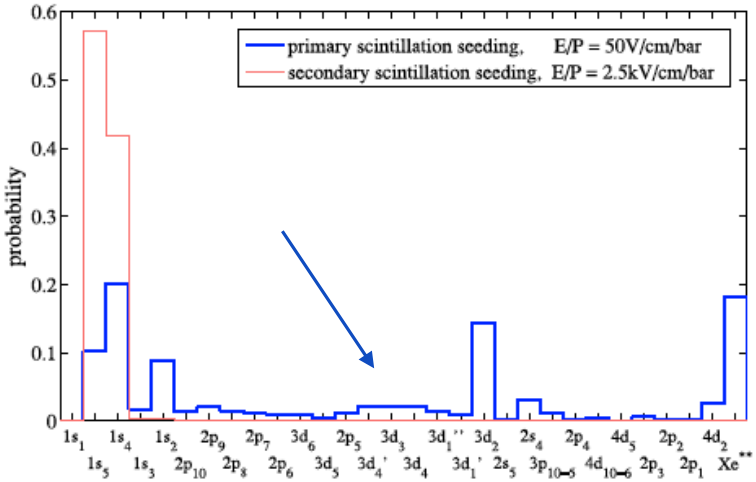
(excited states)

top-down

Low-energy Magboltz cross-sections extended using Born approximation

2.4MeV electron





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```
.........
 ELASTIC ANISOTROPIC     XENON              966443.7699 +-  0.00102 %
 IONISATION CHARGE STATE=1      ELOSS=   12.12984      978.3773 +-  0.03197 %
 IONISATION CHARGE STATE=2      ELOSS=   33.105        82.4206 +-  0.11015 %
 IONISATION CHARGE STATE=3+4+5+6 ELOSS=   64.155       54.8192 +-  0.13506 %
 IONISATION  M5-SHELL           ELOSS=  676.4          2.6195 +-  0.61786 %
 IONISATION  M4-SHELL           ELOSS=  689.0          1.6949 +-  0.76812 %
 IONISATION  M3-SHELL           ELOSS=  940.6          0.6988 +-  1.19625 %
 IONISATION  M2-SHELL           ELOSS= 1002.1          0.2998 +-  1.82635 %
 IONISATION  M1-SHELL           ELOSS= 1148.7          0.1989 +-  2.24224 %
 IONISATION  L3-SHELL           ELOSS= 4786.           0.0563 +-  4.21450 %
 IONISATION  L2-SHELL           ELOSS= 5107.           0.0214 +-  6.83586 %
 IONISATION  L1-SHELL           ELOSS= 5453.           0.0168 +-  7.71517 %
 IONISATION  K-SHELL            ELOSS= 34561.          0.0000 +-  0.00000 %
 ATTACHMENT                                            0.0000 +-  0.00000 %
  EXC  1S5    J=2 METASTABLE   ELOSS=   8.3153        79.9544 +-  0.11184 %
  EXC  1S4    J=1 RESONANT     ELOSS=   8.4365       157.7401 +-  0.07962 %
  EXC  1S3    J=0 METASTABLE   ELOSS=   9.4472        13.3864 +-  0.27332 %
  EXC  1S2    J=1 RESONANT     ELOSS=   9.5697        69.1931 +-  0.12022 %
  EXC  2P10   J=1              ELOSS=   9.5802        10.1655 +-  0.31364 %
  EXC  2P9    J=2              ELOSS=   9.6856        16.5235 +-  0.24601 %
  EXC  2P8    J=3              ELOSS=   9.7207        11.6235 +-  0.29331 %
  EXC  2P7    J=1              ELOSS=   9.7893         8.3640 +-  0.34577 %
  EXC  2P6    J=2              ELOSS=   9.8211         6.2879 +-  0.39879 %
  EXC  3D6    J=0              ELOSS=   9.8904         7.9594 +-  0.35445 %
  EXC  3D5    J=1 RESONANT     ELOSS=   9.9171         3.3748 +-  0.54435 %
  EXC  2P5    J=0              ELOSS=   9.9335         9.3326 +-  0.32734 %
  EXC  3D4!   J=4              ELOSS=   9.9431        15.8000 +-  0.25158 %
  EXC  3D3    J=2              ELOSS=   9.9588        16.8951 +-  0.24329 %
  EXC  3D4    J=3              ELOSS=  10.0391        17.1581 +-  0.24142 %
  EXC  3D1!!  J=2              ELOSS=  10.1575        10.1892 +-  0.31328 %
  EXC  3D1!   J=3              ELOSS=  10.2200         7.0355 +-  0.37701 %
  EXC  3D2    J=1 RESONANT     ELOSS=  10.4010       111.7564 +-  0.09459 %
  EXC  2S5    J=2              ELOSS=  10.5621         1.6939 +-  0.76834 %
  EXC  2S4    J=1 RESONANT     ELOSS=  10.5932        24.1799 +-  0.20336 %
  EXC  SUM 3P10-5              ELOSS=  10.9016         8.6134 +-  0.34073 %
  EXC  2P4    J=1              ELOSS=  10.9576         1.0530 +-  0.97451 %
  EXC  SUM 4D                  ELOSS=  10.9715         4.2233 +-  0.48660 %
  EXC  4D5    J=1 RESONANT     ELOSS=  10.9788         0.2555 +-  1.97836 %
  EXC  2P3    J=2              ELOSS=  11.0547         4.6448 +-  0.46400 %
  EXC  2P2    J=1              ELOSS=  11.0691         1.1447 +-  0.93466 %
  EXC  2P1    J=0              ELOSS=  11.1412         2.1624 +-  0.68004 %
  EXC  4D2    J=1 RESONANT     ELOSS=  11.1626        20.6368 +-  0.22013 %
  EXC  3S4    J=1 RESONANT     ELOSS=  11.2742         5.3803 +-  0.43112 %
  EXC  5D5    J=1 RESONANT     ELOSS=  11.4225         5.2979 +-  0.43446 %
  EXC  5D2    J=1 RESONANT     ELOSS=  11.4951         0.4745 +-  1.45172 %
  EXC  4S4    J=1 RESONANT     ELOSS=  11.5829         0.1169 +-  2.92478 %
  EXC  3S1!   J=1 RESONANT     ELOSS=  11.6072        42.9837 +-  0.15253 %
  EXC  6D5    J=1 RESONANT     ELOSS=  11.6828         1.9538 +-  0.71542 %
  EXC  6D2    J=1 RESONANT     ELOSS=  11.7395        21.2119 +-  0.21713 %
  EXC  5S4    J=1 RESONANT     ELOSS=  11.7521         6.3205 +-  0.39776 %
  EXC  7D5    J=1 RESONANT     ELOSS=  11.8068         0.8992 +-  1.05456 %
  EXC  7D2    J=1 RESONANT     ELOSS=  11.8403        13.4338 +-  0.27284 %
  EXC  6S4    J=1 RESONANT     ELOSS=  11.8518         0.5402 +-  1.36058 %
  EXC  2S2    J=1 RESONANT     ELOSS=  11.8778         6.2008 +-  0.40158 %
  EXC  8D5    J=1 RESONANT     ELOSS=  11.8917         0.7586 +-  1.14814 %
  EXC  8D2    J=1 RESONANT     ELOSS=  11.9082         8.2060 +-  0.34909 %
  EXC  7S4    J=1 RESONANT     ELOSS=  11.9177         1.0675 +-  0.96787 %
  EXC  9D5    J=1 RESONANT     ELOSS=  11.9416         0.1037 +-  3.10535 %
  EXC  9D2    J=1 RESONANT     ELOSS=  11.9550         5.3311 +-  0.43310 %
  EXC  8S4    J=1 RESONANT     ELOSS=  11.9621         0.4888 +-  1.43032 %
  EXC  10D5   J=1 RESONANT     ELOSS=  11.9789         0.1075 +-  3.04997 %
  EXC  10D2   J=1 RESONANT     ELOSS=  11.9886         3.4669 +-  0.53707 %
  EXC  9S4    J=1 RESONANT     ELOSS=  11.9939         0.2995 +-  1.82727 %
  EXC  HIGH   J=1 RESONANT     ELOSS=  12.0           17.4430 +-  0.23944 %
.........
```

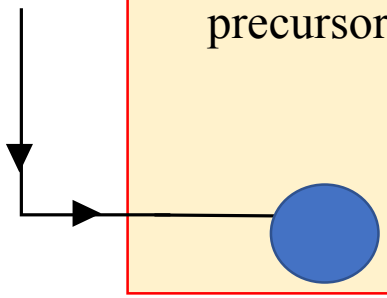
atomic cascade: radiative and radiationless (collisional) decays

xenon

State (Paschen)[a]	State (Racah)[b]	Energy [eV]	$1/\tau=\sum_j A_{ij}$ [ns^{-1}]	K_2@1bar [ns^{-1}]
$1s_1$	–	0.000	–	–
$1s_5$	$6s[3/2]_2$	8.315	2.33×10^{-11}	4.94×10^{-5}
$1s_4$	$6s[3/2]_1$	8.437	$0.281/n_H$	–
$1s_3$	$6s'[1/2]_0$	9.447	1.28×10^{-8}	0.2224
$1s_2$	$6s'[1/2]_1$	9.570	$0.246/n_H$	2.4954
$2p_{10}$	$6p[1/2]_1$	9.580	0.026	3.7802
$2p_9$	$6p[5/2]_2$	9.686	0.027	2.7425
$2p_8$	$6p[5/2]_3$	9.721	0.031	1.8036

ransfer precursors

III. Transfer precursor



characteristics of atomic cascade:

1. time-scale:

$$\tau^* \simeq \frac{\tau}{1+\tau K_2} = \mathbf{30}\ \ \mathbf{ns}\ \ (\mathbf{P} \lesssim 1\ \mathbf{mbar})$$

radiation dominated

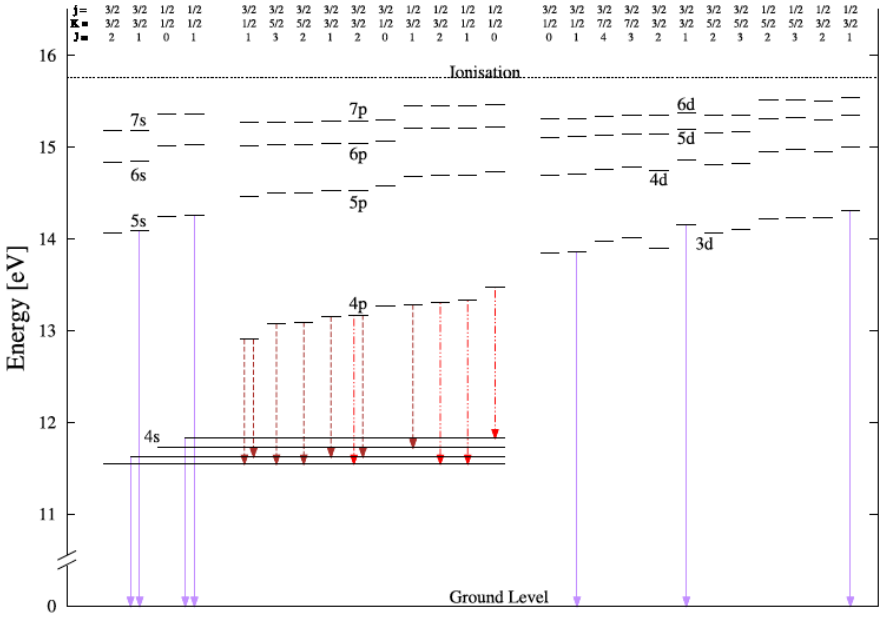
$$\tau^* \simeq \frac{\tau}{1+\tau K_2} = 0.1\text{–}1\ \text{ns}\ \ (\mathrm{P} \gtrsim 1\ \text{bar})$$

collision dominated

2. transfer probability during cascade:

transfer rates are ns-scale at 1bar (e.g., if using a simple solid-sphere calculation). So transfer-reactions from high-lying states are highly suppressed.

argon



scintillation vs quenching

radiative decay competes with transfer at this point (except for metastable states)

State (Paschen)[a]	State (Racah)[b]	Energy [eV]	$\sum_j A_{ij}$ [ns^{-1}]	K_2@1bar [ns^{-1}]
$1s_1$	–	0.000	–	–
$1s_5$	$6s[3/2]_2$	8.315	2.33×10^{-11}	4.94×10^{-5}
$1s_4$	$6s[3/2]_1$	8.437	$0.281/n_H$	–
$1s_3$	$6s'[1/2]_0$	9.447	1.28×10^{-8}	0.2224
$1s_2$	$6s'[1/2]_1$	9.570	$0.246/n_H$	2.4954
$2p_{10}$	$6p[1/2]_1$	9.580	0.026	3.7802

metastable

resonant

number of absorption-emission cycles increases with P·L

$$n_c \simeq 0.87(3\pi^2 \frac{\varepsilon_0}{hc} PL)^{1/2}$$

~1000 for ~1bar cm

τ_{s4} = 4.5ns -> 4.5μs!

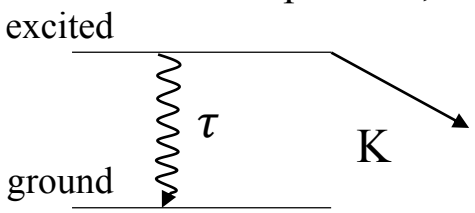
transfers do *not* require of metastable states to be the precursors:

1) Resonant states play the role, too, due to resonant-trapping.
2) Resonant transfer can even outcompete a fast decay rate.

λ_1

IV. Scintillation probability (P_{scin})

simple case, for illustration



$$\frac{dN_{ex}}{dt} = (\frac{1}{\tau} + K) \cdot N_{ex}$$

$$N_{ex}(t) = N_{ex,0} \cdot e^{-t/\tau^*}$$

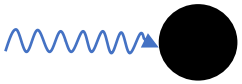
$$\frac{1}{\tau^*} = \frac{1}{\tau} + K$$

$$P_{scin} = \frac{\tau^*}{\tau}$$

Stern-Vollmer relations

photoabsorption and re-emission

example 1
absorption of xenon light by common species



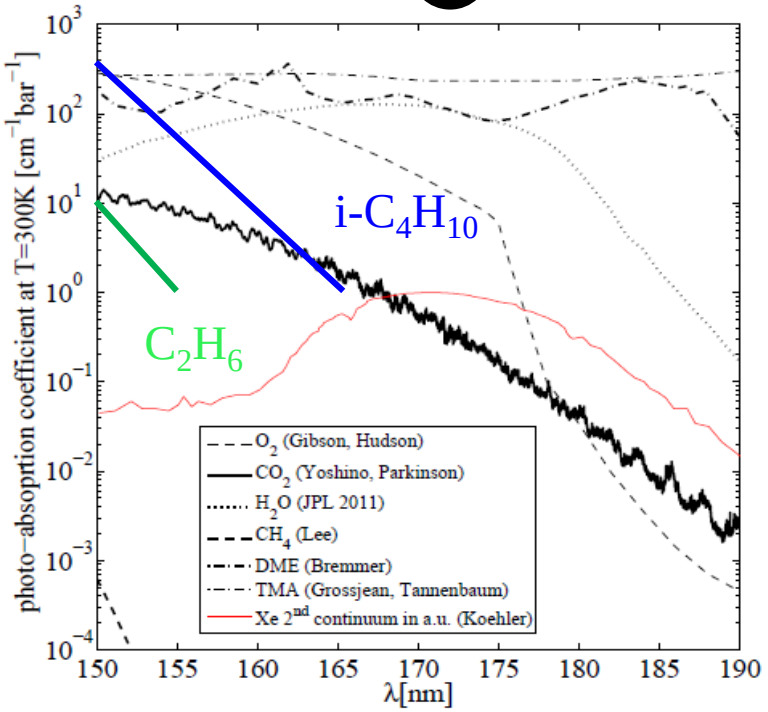
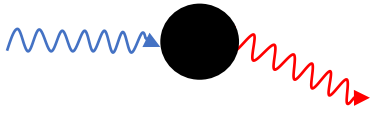


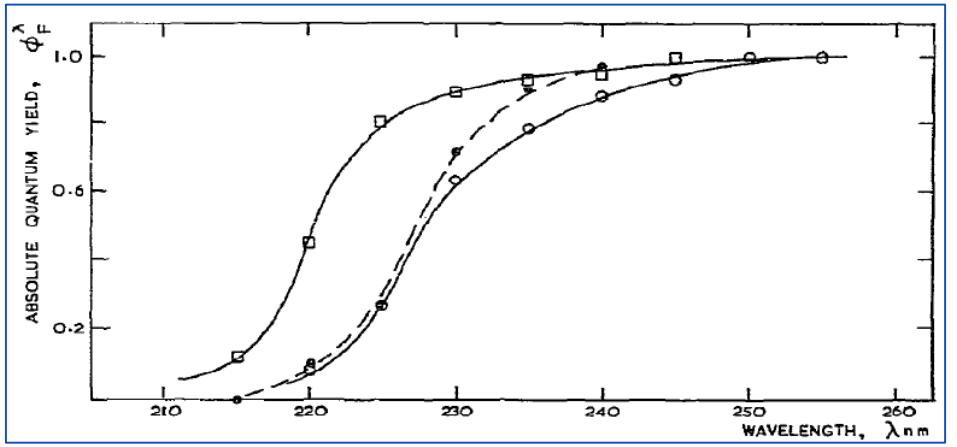
Fig. 1. Compilation of photo-absorption coefficients of some relevant TPC admixtures at around $T = 300$K in the region corresponding to the Xenon 2nd continuum, [9–18]. The reference spectrum from Koehler has been overlaid as a thin continuous line [2]. For H_2, N_2 and CF_4 there is no data in the region shown, and their cross-sections are plausibly orders of magnitude below that of CH_4.

$$\Pi = \frac{1}{P}\frac{N}{V}\sigma_{pa} \qquad \mathcal{T}(z) = \frac{\int \frac{dN_\gamma}{d\lambda} e^{-\Pi(\lambda)z} d\lambda}{\int \frac{dN_\gamma}{d\lambda} d\lambda}$$

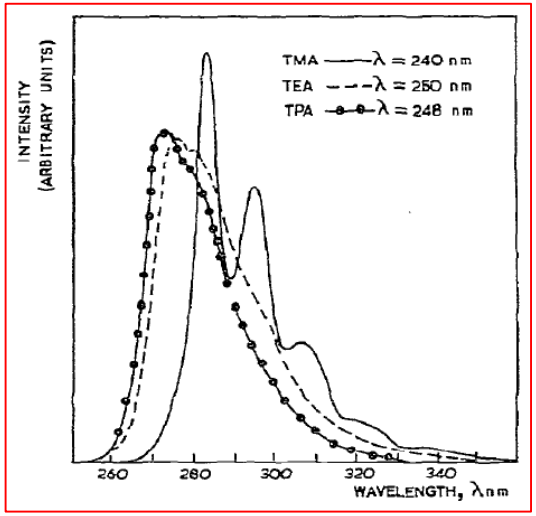
http://satellite.mpic.de/spectral_atlas

example 2
TMA fluorescence

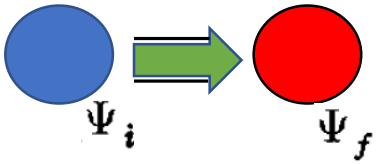




λ_1
V. Photoabsorption



transfer reactions



Several mechanisms available, in the simplest case, Fermi golden rule may be applied

$$k(t) = (2\pi/h)\rho(E)\left|\langle\Psi_f\left|V\right|\Psi_i\rangle\right|^2$$

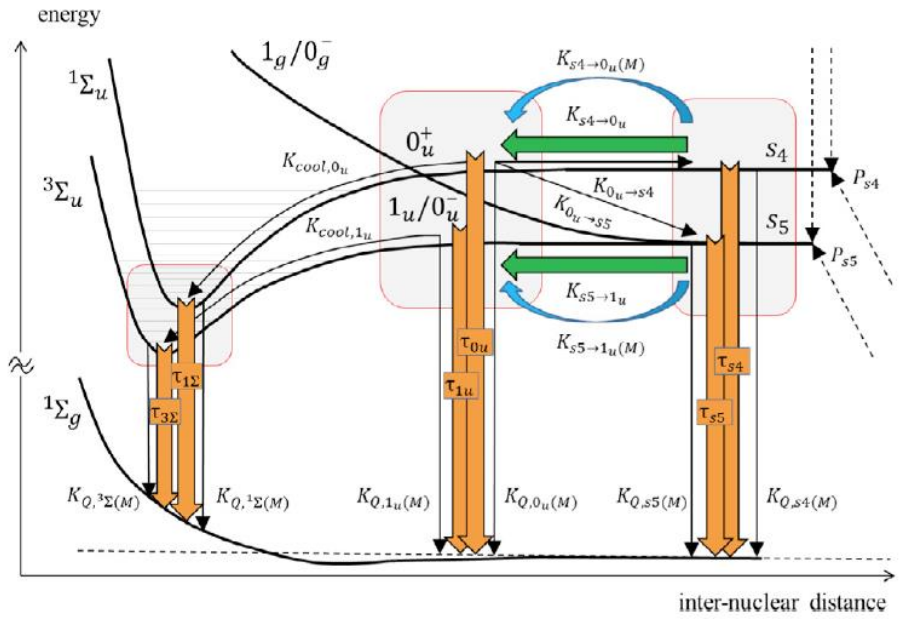
density of product states — final state — dipole-dipole potential — initial state

$E^* + BC$	$\rightarrow E + BC^+ + e^-$	Penning effect
	$\rightarrow (EBC)^+ + e^-$	associative ionization
	$\rightarrow E + B^+ + C^-$	pair formation
	$\rightarrow E + BC^*$	excitation transfer
	$\rightarrow E + B + C$	dissociation
	$\rightarrow E + B^* + C \quad (C^* + B)$	dissociative excitation
	$\rightarrow EB^* + C \quad (EC^* + B)$	reactive quenching (to excited state)
	$\rightarrow EB + C \quad (EC + B)$	reactive quenching (to ground state)

VI. Transfer

Most information is **experimental**, however, highlighting the role of:

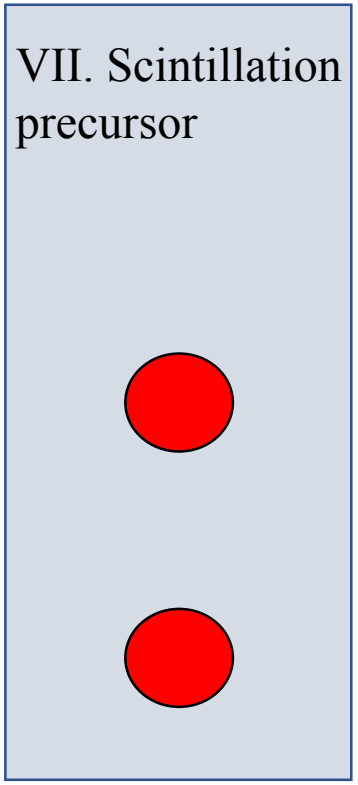
- Polarizability (or permanent dipole moment).
- Atom/Molecule Size.
- Difference in energy between initial and final excited states.



precursors

A common characteristic of the scintillation precursor is that it will wavelength-shift scintillation with respect to the natural one of the directly-excited species (this shift will make the medium self-transparent to its own fluorescence -> Stokes shift!)

- Excimer formation in noble gases (NG_2^*) leads to a small shift in scintillation by about 0.5eV.
- Tertiary amines change shape when promoted to the first excited state, leading to about 1eV shift between absorption and emission.
- CF_4 fragments into CF_3^* and CF_4^{+*}, with CF_4 being transparent to their emission.



towards the microscopic modelling scintillation-based TPCs (why?)

Some experimental information on the scintillation characteristics of a given gas mixture will be needed, in general, so what modelling is good for?:

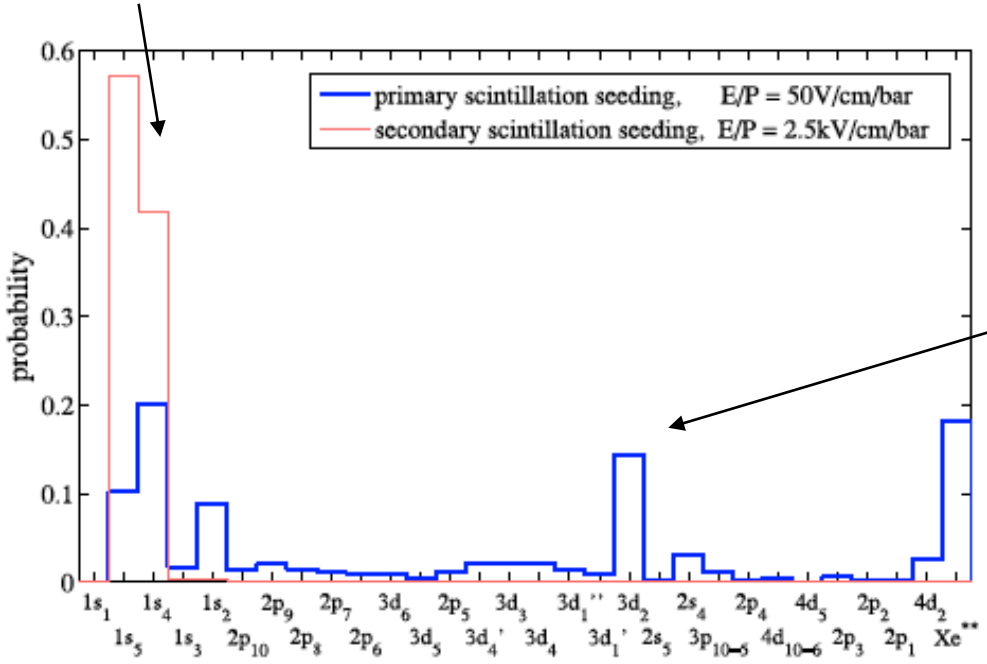
- Modelling allows **extrapolation to different N-density conditions** ($N = P/k_BT$).
- It **allows obtaining** some **information about primary scintillation** (more difficult to measure), **starting from secondary scintillation. And viceversa.** For instance, through the estimate of the scintillation probability of a mixture (P_{scin}).
- **Effect of a third species**, necessary for drift-diffusion tuning of a TPC becomes **very easy to evaluate.**
- **It allows educated guesses**. For the most studied gases (e.g., nobles), predictions relying on the existing (vast) photochemical information are possible.
- Experimental information about absolute scintillation yields, can be bootstrapped, with the help of the model, to obtain **detailed spectroscopic information and time dependences**.
- This detailed understanding is **essential in order to attempt to model other processes, such as photon-driven streamer formation**.

Main deliverables:

- Estimates of **W_{sc}-values** (average energy to create a photon) for each relevant band.
- Estimates of **secondary scintillation yields**, for each relevant band.
- **Time and spectral information**.

input to simulation (distribution of excited states) -> xenon as an example!

secondary scintillation:
electron transport software (Garfield++, Magboltz, Pyboltz)



primary scintillation: (Degrad)

Fig. 1. Simulated probability distributions for the first 41 excited states of xenon upon interaction of a 30 keV electron. The primary scintillation seeding (thick lines) refers to the case where the excited states are directly promoted by the impinging electron; in the secondary scintillation case the seeding is generated by the ionization electrons, with assistance from an external field at a convenient location (thin lines).

input to scintillation model (atomic cascade *in pure gas*)

I. Transition probabilities (collisional & radiative)

State (Paschen)[a]	State (Racah)[b]	Energy [eV]	$\sum_j A_{ij}$ [ns^{-1}]	K_2@1bar [ns^{-1}]	K_3@1bar [ns^{-1}]
$1s_1$	–	0.000	–	–	–
$1s_5$	$6s[3/2]_2$	8.315	2.33×10^{-11}	4.94×10^{-5}	0.1465
$1s_4$	$6s[3/2]_1$	8.437	$0.281/n_H$	–	0.0855
$1s_3$	$6s'[1/2]_0$	9.447	1.28×10^{-8}	0.2224	–
$1s_2$	$6s'[1/2]_1$	9.570	$0.246/n_H$	2.4954	–
$2p_{10}$	$6p[1/2]_1$	9.580	0.026	3.7802	–
$2p_9$	$6p[5/2]_2$	9.686	0.027	2.7425	–
$2p_8$	$6p[5/2]_3$	9.721	0.031	1.8036	–
$2p_7$	$6p[3/2]_1$	9.789	0.028	4.3979	–
$2p_6$	$6p[3/2]_2$	9.821	0.036	2.0062	–
$3d_6$	$5d[1/2]_0$	9.890	4.36×10^{-3}	9.7649	–
$3d_5$	$5d[1/2]_1$	9.917	$0.015/n_H$	4.8328	–
$2p_5$	$6p[1/2]_0$	9.933	0.031	0.1599	0.4273
$3d'_4$	$5d[7/2]_4$	9.943	4.34×10^{-3}	4.8676	–
$3d_3$	$5d[3/2]_2$	9.959	8.16×10^{-3}	4.8664	–
$3d_4$	$5d[7/2]_3$	10.039	7.34×10^{-3}	4.8510	–
$3d''_1$	$5d[5/2]_2$	10.157	1.21×10^{-3}	4.8649	–
$3d'_1$	$5d[5/2]_3$	10.220	1.39×10^{-3}	4.8639	–
$3d_2$	$5d[3/2]_1$	10.401	$3.04\times10^{-3}/n_H$	1.3637	–
$2s_5$	$7s[3/2]_2$	10.562	0.018	4.9415	–
$2s_4$	$7s[3/2]_1$	10.593	$0.178/n_H$	4.9415	–
$3p_{10-5}$[c]	–	10.902	0.010	12.6008	–
$2p_4$	$6p[3/2]_1$	10.958	0.024	10.3277	–
$4d_{10-6,4,3}$[d]	–	10.971	0.014	5.9298	–
$4d_5$	$6d[1/2]_1$	10.979	0.018	4.8426	–
$2p_3$	$6p[3/2]_2$	11.055	0.036	11.6125	–
$2p_2$	$6p[1/2]_1$	11.069	0.033	10.3277	–
$2p_1$	$6p[1/2]_0$	11.141	0.027	10.4018	–
$4d_2$	$6d[3/2]_1$	11.163	$0.716/n_H$	4.8674	–
Xe**	–	11.7	–	12.35	–

3-body collisional quenching (excimer formation)

2-body collisional quenching (excimer formation)

decay rate

II. Decay probability matrixes (collisional & radiative)

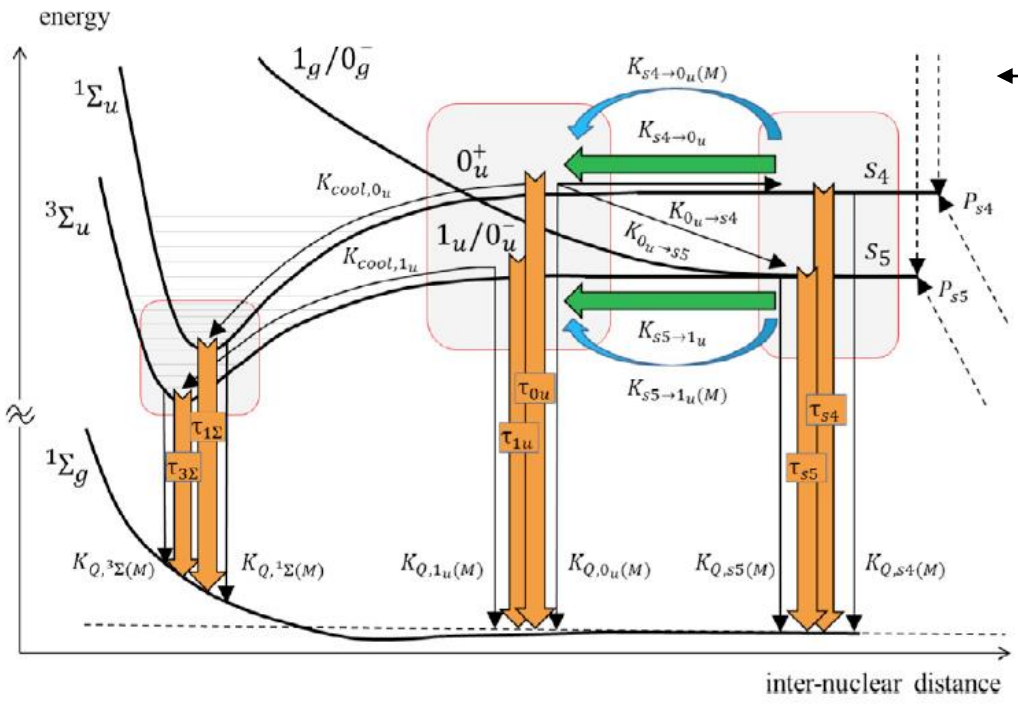
–	$1s_1$	$1s_5$	$1s_4$	$1s_3$	$1s_2$	$2p_{10}$	$2p_9$	$2p_8$	$2p_7$	$2p_6$	...
$1s_1$	–	0	0	0	0	0	0	0	0	0	
$1s_5$	$1^{(1)}$	–	0	0	0	0	0	0	0	0	
$1s_4$	0	0	–	0	0	0	0	0	0	0	
$1s_3$	0	$0.11^{(2,3)}$	$0.89^{(2,3)}$	–	0	0	0	0	0	0	
$1s_2$	0	$0.010^{(2,3)}$	$0.079^{(2,3)}$	$0.247^{(3)}$	–	$0.663^{(4)}$	0	0	0	0	
$2p_{10}$	0	$0.014^{(3)}$	$0.116^{(3)}$	$0.216^{(4)}$	$0.654^{(4)}$	–	0	0	0	0	
$2p_9$	0	0	0	$0.3604^{(4)}$	$0.1351^{(3)}$	$0.405^{(4)}$	–	$0.099^{(4)}$	0	0	
$2p_8$	0	0	0	$0.178^{(3)}$	$0.110^{(3)}$	$0.245^{(3)}$	$0.466^{(3)}$	–	0	0	
$2p_7$	0	0	0	$0.348^{(3)}$	$0^{(2)}$	$0.011^{(2)}$	$0.067^{(2)}$	$0.539^{(2)}$	–	$0.034^{(3)}$	
$2p_6$	0	0	0	$0.234^{(3)}$	$0.001^{(2)}$	$0.001^{(2)}$	$0.345^{(3)}$	$0.259^{(3)}$	$0.161^{(3)}$	–	
⋮											

collisional decay matrix

C. Azevedo, D. Gonzalez-Diaz, et al., Microscopic simulation of xenon-based optical TPCs in the presence of molecular additives, Nucl. Instrum. Methods. Phys. Res. A 877 (2018) 157.

input to scintillation model (transfers leading to scintillation precursors in *pure gas*)

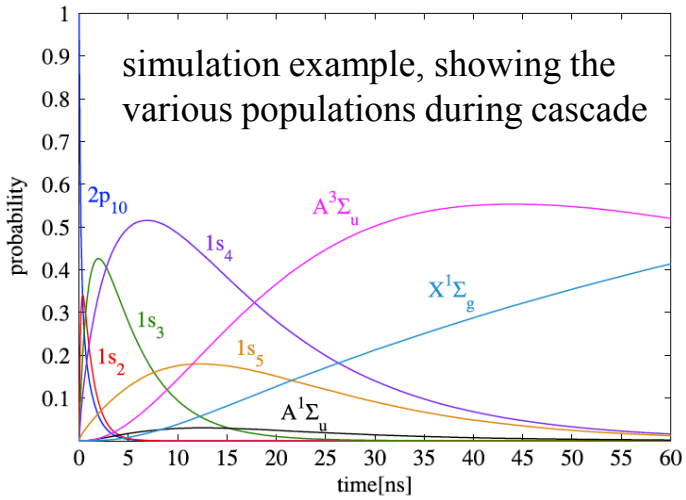
III. Formation of scintillation precursors & decay



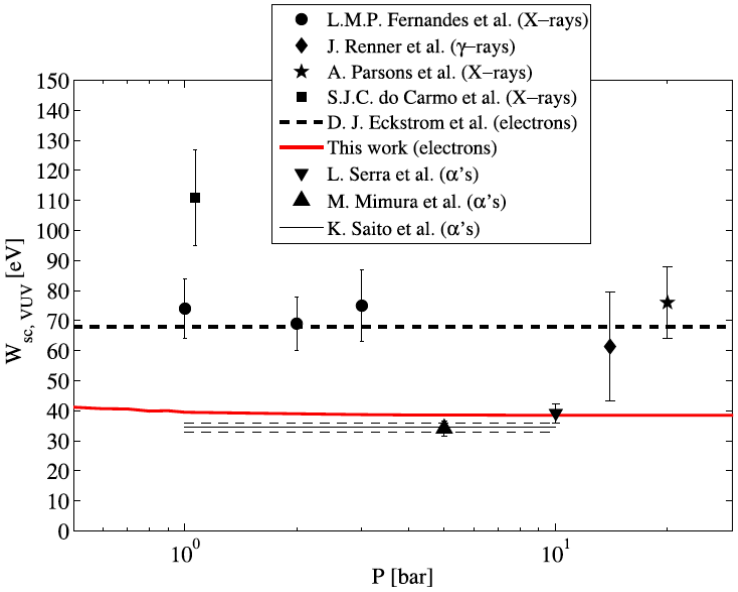
general diagram in noble gases (sometimes called Wenck scheme)

also included in matrix form

$\tau_{3\Sigma}$ [a]	100 ns[(1)]	$K_{s_5\to 1_u}$	0.1465 ns^{-1}[(1)]
$\tau_{1\Sigma}$	4.55 ns[(1)]	$K_{s_4\to 0_u}$	0.0855 ns^{-1}[(1)]
τ_{1_u} [b]	40 ns[(1)]	$K_{0_u\to s_4}$	1.43 ns^{-1}[(1)]
τ_{0_u}	5 ns[(1)]	$K_{0_u\to s_5}$	6.42 ns^{-1}[(1)]
τ_{s_5}	42 s[(2)]	$K_{cool,0_u}$	1.72 ns^{-1}[(1)]
τ_{s_4}	$3.56\times n_H$ ns[(3)]	$K_{cool,1_u}$	1.72 ns^{-1}[(1)]



yields

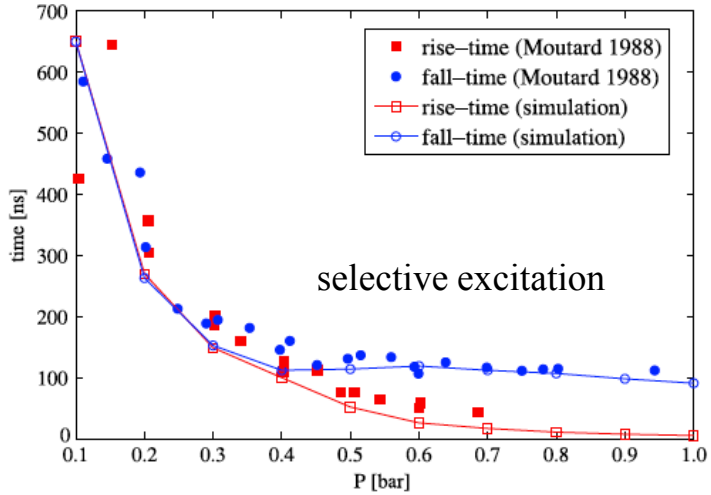


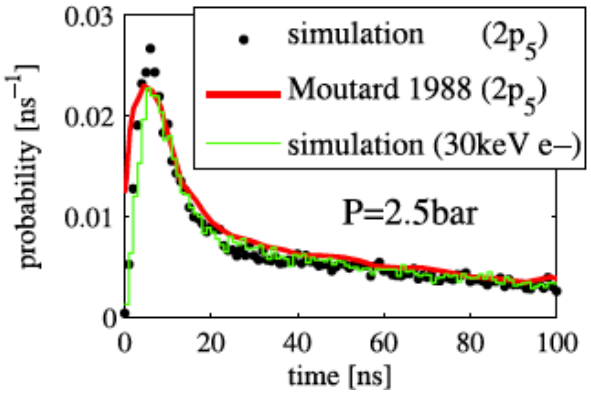
$W_{sc,IR} = 86$ eV (simulated)

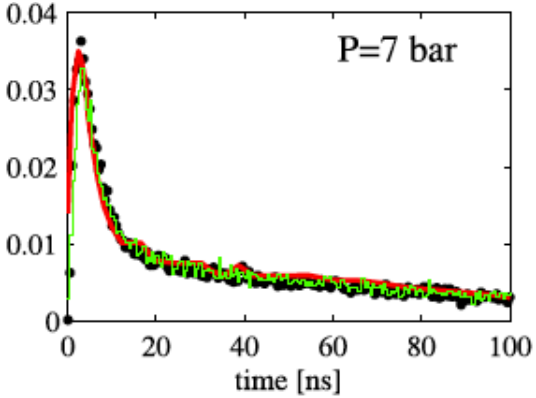
$W_{sc,IR} \lesssim 48 \pm 7$ eV (measured)

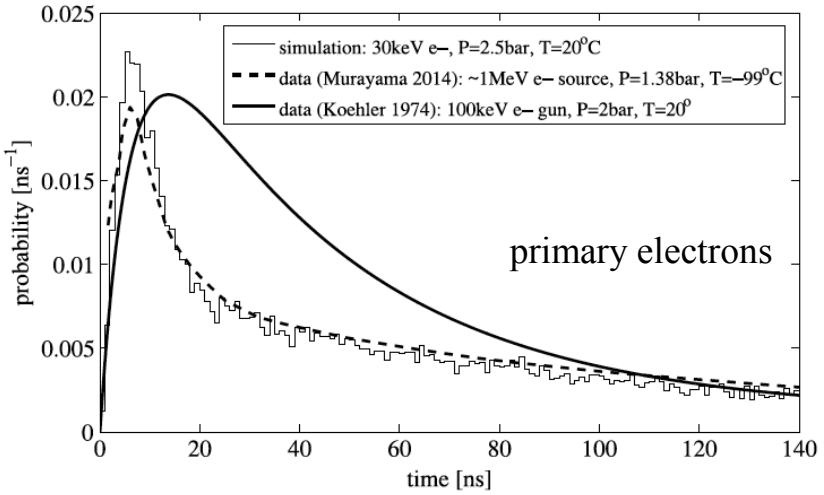
benchmark (*pure gas*)

temporal spectra









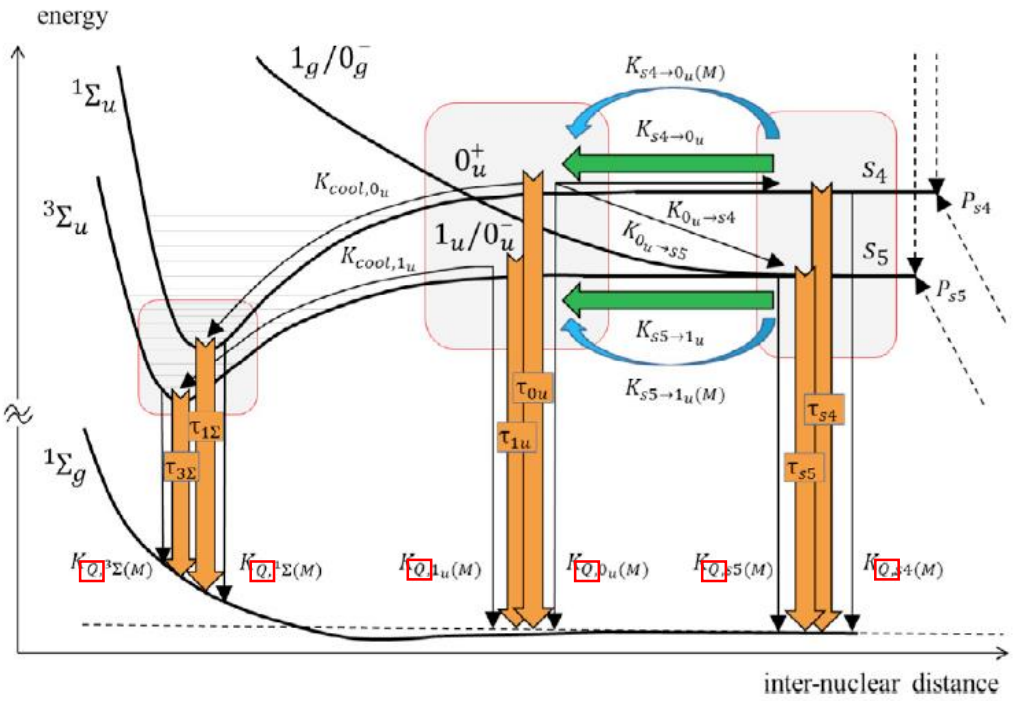
input to simulation (transfers leading to scintillation precursors in a *xenon mixtures*)

IV. Cascade quenching by additives (only collisional)

State (Paschen)[a]	K_2@1bar [ns^{-1}]
$1s_1$	
$1s_5$	
$1s_4$	
$1s_3$	
$1s_2$	
$2p_{10}$	
$2p_9$	
$2p_8$	
$2p_7$	
$2p_6$	
$3d_6$	
$3d_5$	
$2p_5$	
$3d'_4$	
$3d_3$	
$3d_4$	
$3d''_1$	
$3d'_1$	
$3d_2$	
$2s_5$	
$2s_4$	
$3p_{10-5}$[c]	
$2p_4$	
$4d_{10-6,4,3}$[d]	
$4d_5$	
$2p_3$	
$2p_2$	
$2p_1$	
$4d_2$	
Xe**	

replace for each species (uncertainties here are much larger than for pure gas, fortunately the effect is subdominant for small concentrations of additive)

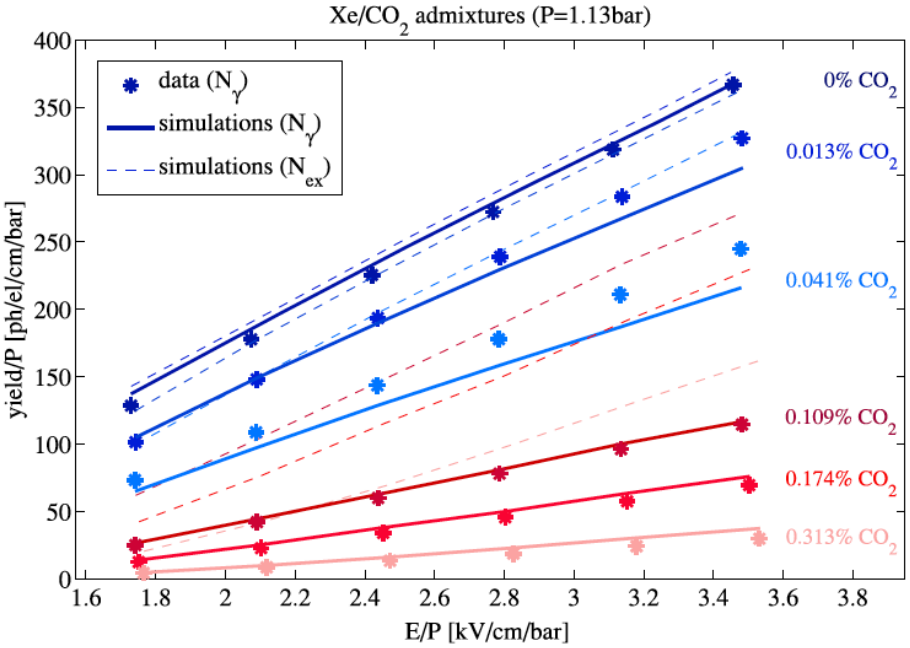
V. Quenching of scintillation precursors by additives

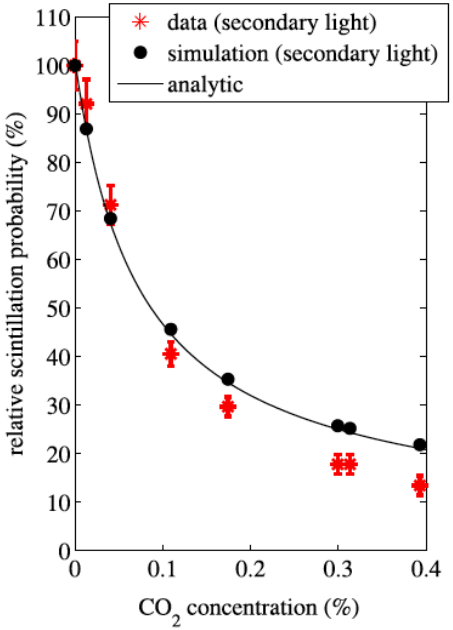


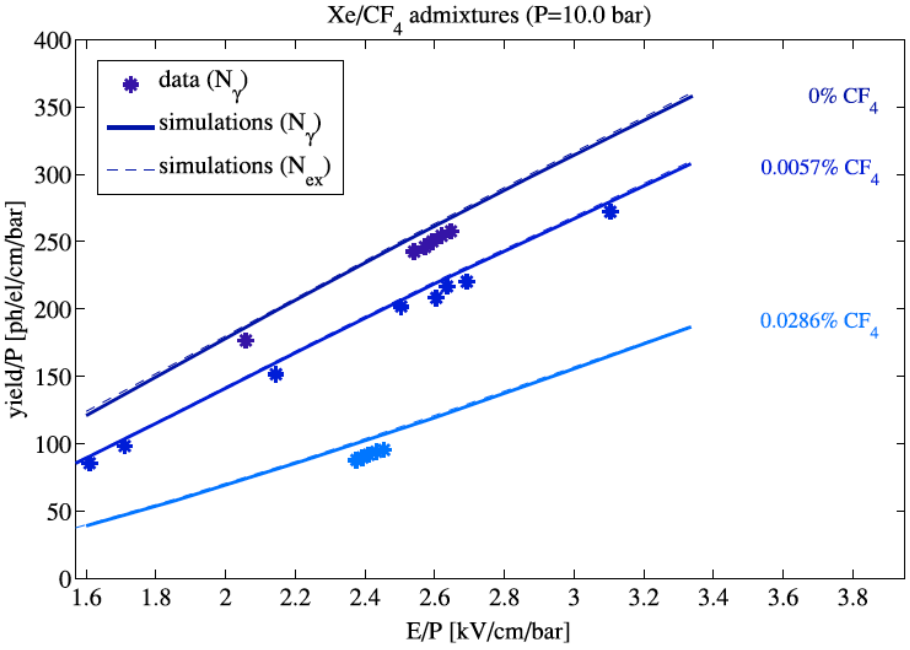
$\tau_{3\Sigma}$[a]	100 ns[(1)]	$K_{Q,^3\Sigma(M)}$	11.12 ns^{-1}
$\tau_{1\Sigma}$	4.55 ns[(1)]	$K_{Q,^1\Sigma(M)}$	12.85 ns^{-1}
τ_{1_u}[b]	40 ns[(1)]	$K_{Q,1_u(M)}$	11.12 ns^{-1}
τ_{0_u}	5 ns[(1)]	$K_{Q,0_u(M)}$	12.85 ns^{-1}
τ_{s_5}	42 s[(2)]	$K_{Q,s_5(M)}$	11.12 ns^{-1}[(4)]
τ_{s_4}	3.56 × n_H n	$K_{Q,s_4(M)}$	12.85 ns^{-1}[(5)]

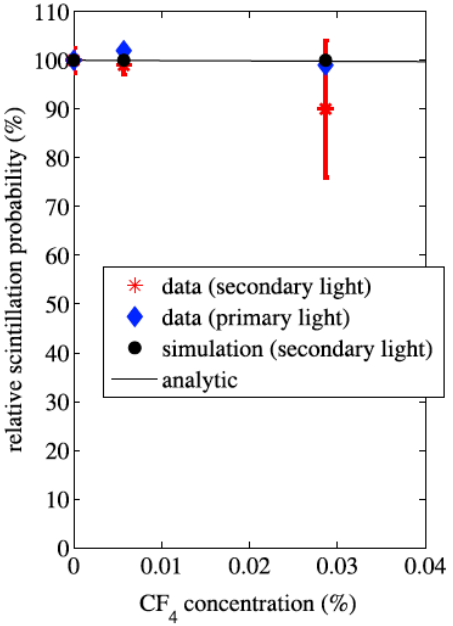
(example for CO_2)

benchmark (*gas mixtures*)

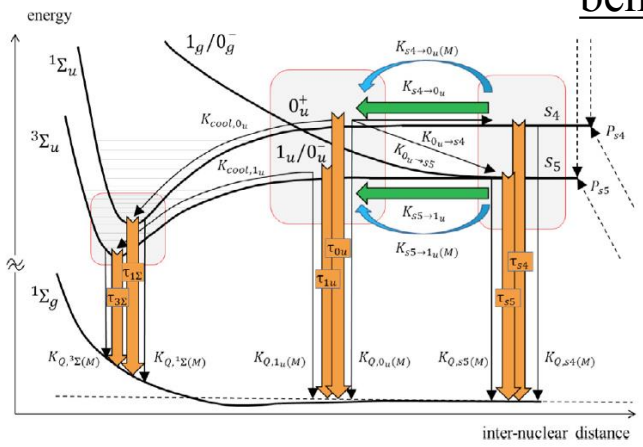








benchmark (*gas mixtures*)



$$\mathcal{P}_{scin,s_4} = \frac{\mathcal{P}_{pop,s_4} \cdot \mathcal{P}_{s_4 \to 0_u}}{1 - \mathcal{P}_{s_4 \to 0_u} \cdot \mathcal{P}_{0_u \to s_4}} \times \left(\mathcal{P}_{cool,0_u} \cdot \mathcal{P}_{rad,^1\Sigma} + \mathcal{P}_{0_u \to s_5} \cdot \mathcal{P}_{s_5 \to 1_u} \cdot \mathcal{P}_{cool,1_u} \cdot \mathcal{P}_{rad,^3\Sigma} \right)$$

$$\mathcal{P}_{scin,s_5} = \mathcal{P}_{pop,s_5} \cdot \mathcal{P}_{s_5 \to 1_u} \cdot \mathcal{P}_{cool,1_u} \cdot \mathcal{P}_{rad,^3\Sigma}$$

It is in fact possible in this case to obtain a simple expression

fraction of singlet (from MC) — fraction of triplet (from MC)

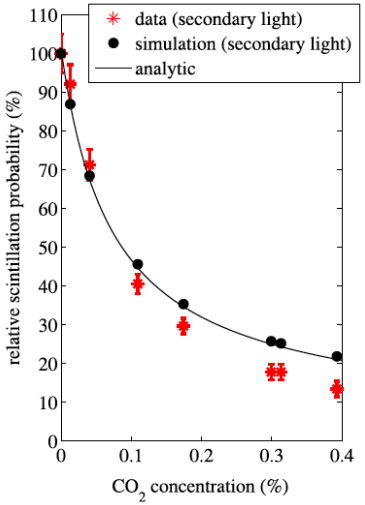
$$\mathcal{P}_{scin} \simeq \frac{F_1}{1 + f \cdot n \cdot \tau_{1_\Sigma} \cdot K_{Q,^1\Sigma}} + \frac{F_3}{1 + f \cdot n \cdot \tau_{3_\Sigma} \cdot K_{Q,^3\Sigma}}$$

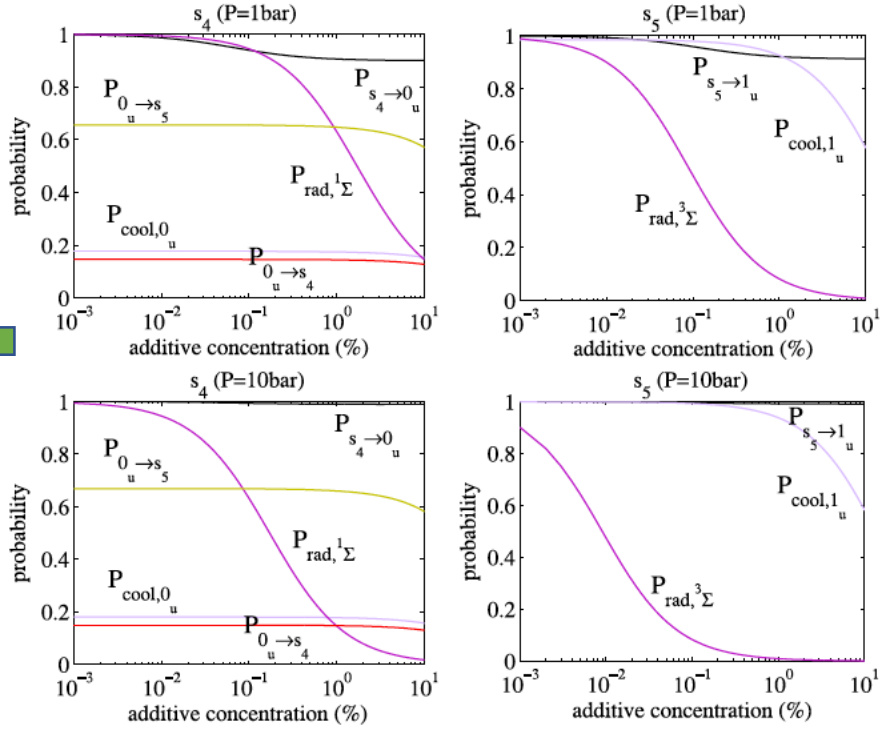
fraction of additive

pressure increase

quenching rate

time constant singlet





conclusions

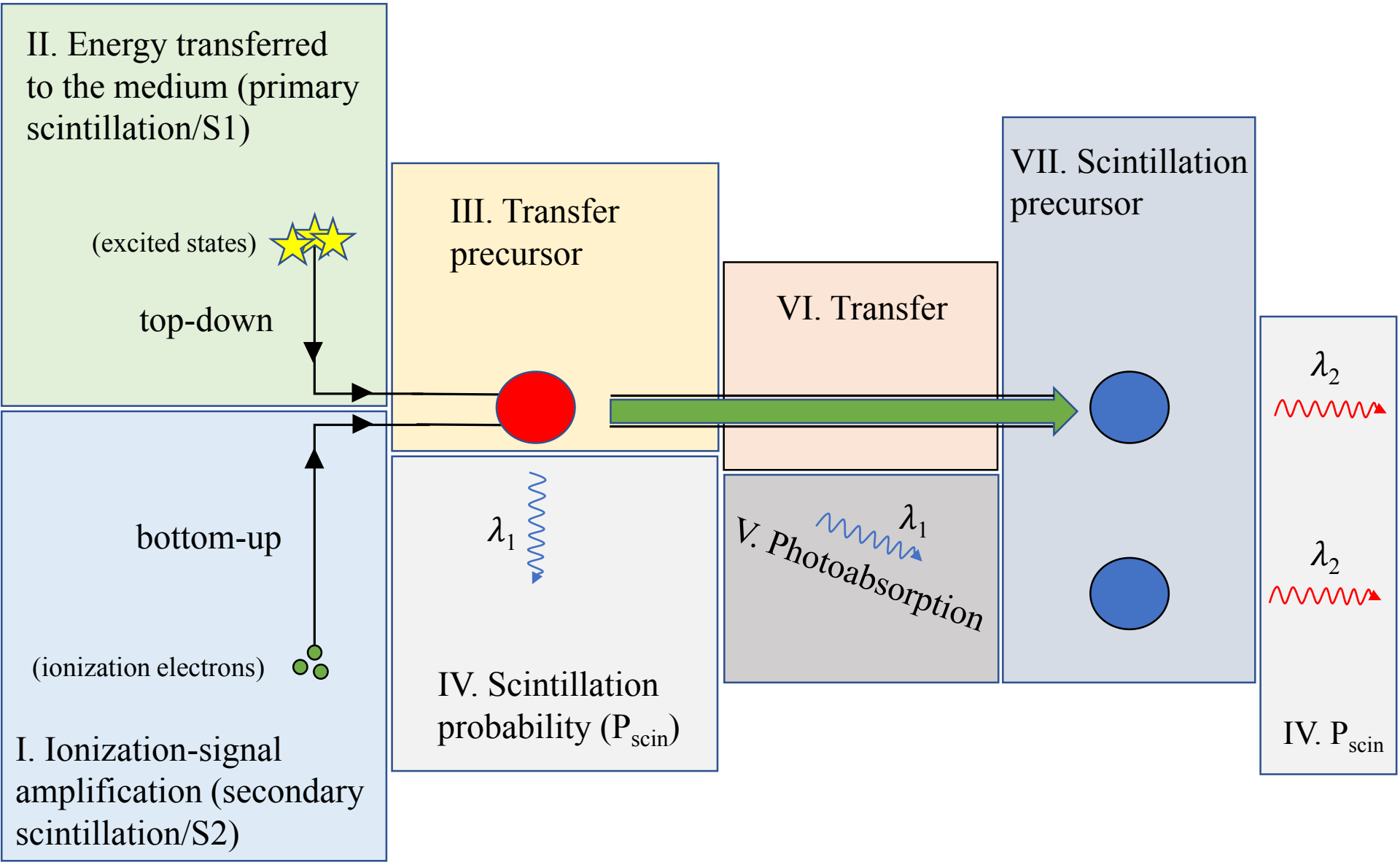
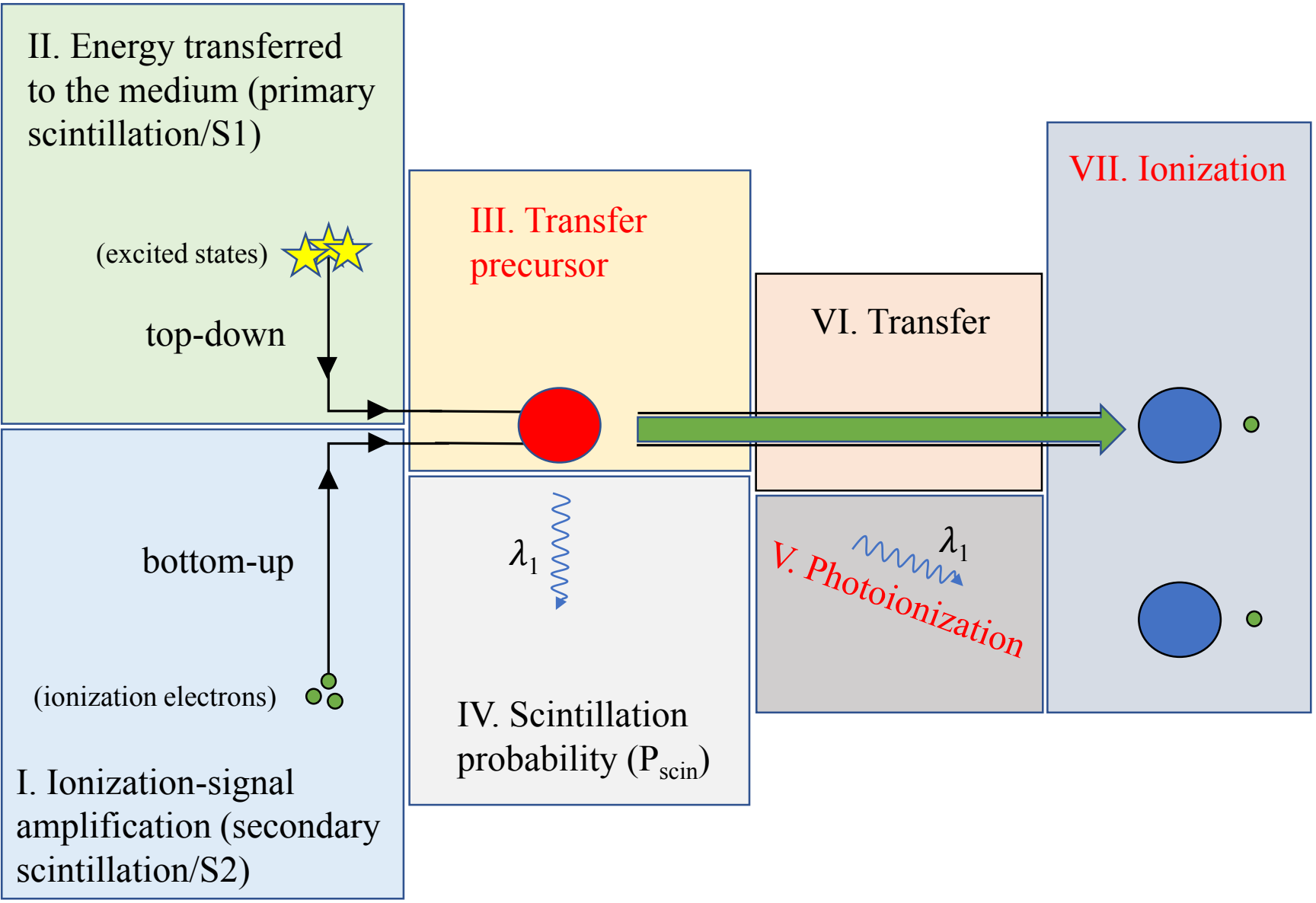
- The understanding of the scintillation in gases is essential for next-generation optical and electroluminescence TPCs.
- In particular, addressing the role of transfer reactions requires a detailed microscopic approach, including the atomic cascade. The TPC ‘chemistry’ needs to be implemented in detail!.
- Modelling of scintillation in xenon (and its mixtures) achieved, displays good quantitative description of existing data. This has been extremely useful as part of the NEXT R&D program.

scope

- Finalize experimental campaign with xenon mixtures and do full benchmark (includes systematics with new additives, nBr, and third continuum). Close the xenon + X case.
- Porting of algorithms and tables to Pyboltz already started.
- Include Argon and Krypton atomic cascade and excimer formation.
- Include Argon-mixtures (of interest to the ND-GAr TPC intended for DUNE).

- Adapt to Penning calculations?.

How scintillation operates at 'high' pressures (>100mbar)



A very similar scheme applies to Penning transfers too!