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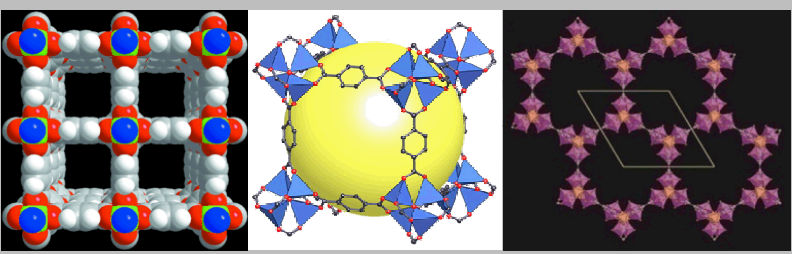

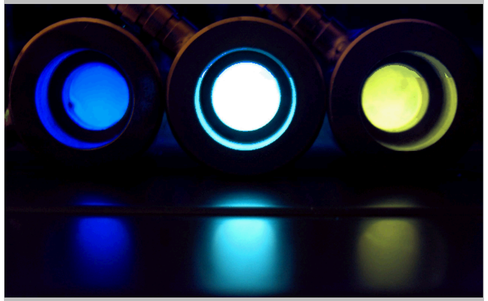

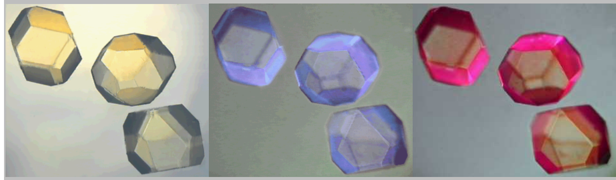

Particle Discrimination Using Nanoporous Metal-Organic Frameworks

SORMA West 2012

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U.S. DEPARTMENT OF ENERGY

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Introduction

- Fast Gamma / Neutron particle discrimination
- PSD (1950's)
  - Molecular Organic Scintillators: **Original PSD**
    - – Most crystallize in non-cubic space groups; necessitates large single crystals
    - – Mechanically fragile ; susceptible to radiation induced damage
    - – Difficult to control luminescent properties systematically

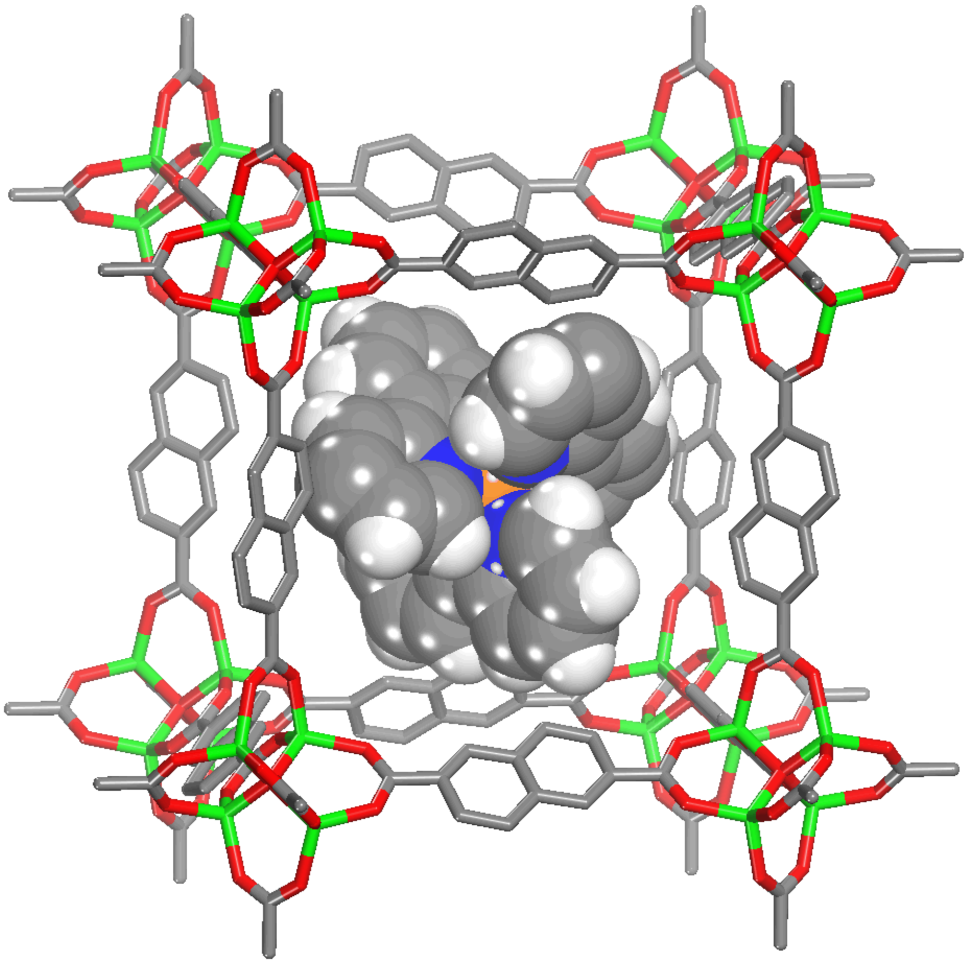
    Zaitseva, N. *et al., IEEE Trans. Nucl. Sci.,* **2011,** *58*(6), 3411-3420.
  - Liquid Scintillators
    - – toxic; highly flammable; scalability and transportation problems;
  - Plastic Scintillators
    - – Cheap, solid material; good for large volume needs
    - – Until recently did not exhibit PSD

    Zaitseva, N. *et al., Nucl. Instr. Meth. A,* **2012**, *668*, 88-93.

    Feng, P.F. *et al., IEEE Trans. Nucl. Sci., Submitted 2012*

What are Metal-Organic Frameworks ?

- Crystalline materials
- Permanent nanoporosity
- > 10,000 unique structures
- Cubic crystal structures
- Strong coordinate covalent bonding

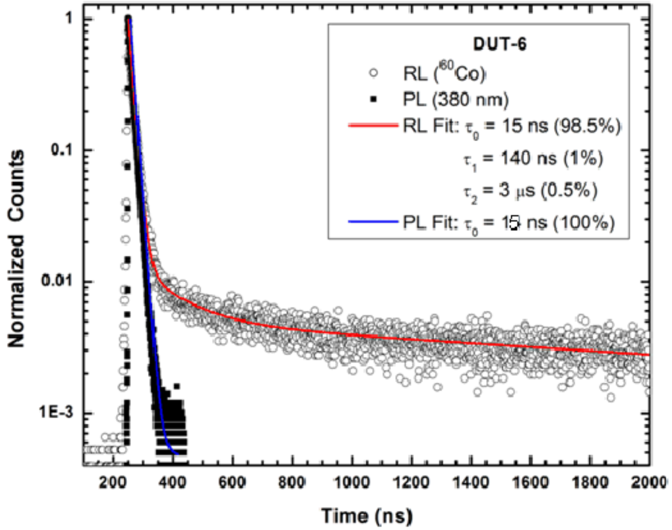


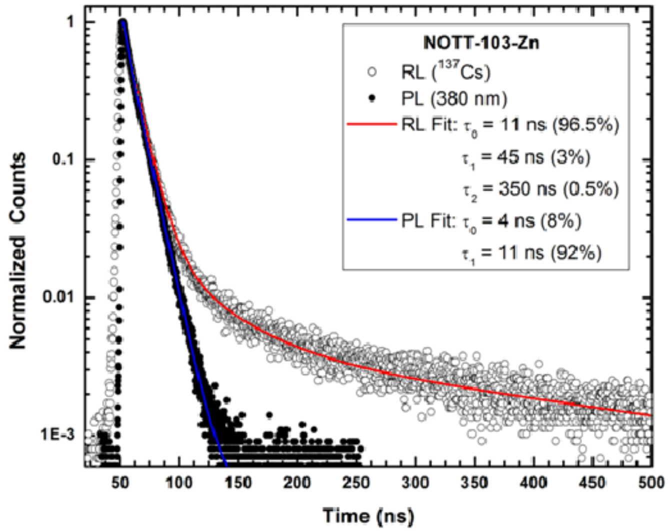
MOF Scintillation

- ***Tunable luminescence decay times***: 1 – 15 ns (prompt); 40 – 3000 ns (delayed)
- ***Light yield***: as much as 98% of anthracene in a MOF+TH hybrid (62% of anthracene in the MOF alone).
- ***H:C ratio***: up to 1.46 in a MOF alone (4.8×10^{22} H cm^{-3}); as high as 1.98 if the pores are filled with H_2 gas
- ***Resistant to radiation induced damage***
- ***Gamma rejection* (PSD)**: 1×10^{-3}
- ***Gamma-neutron* FOM (SSD)**: 4
- ***Gamma-neutron* FOM (PSD)**: 1.3

Tailored Scintillation Decay

- Closed-Shell metal cations
- Isolate emission to linker
- Unique Topological Structure
- Spatially control organic moieties: linker-linker distance and orientation

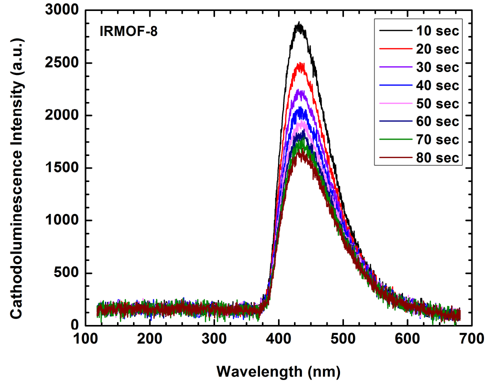


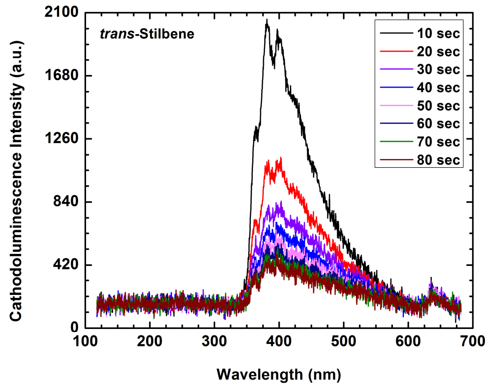


Perry IV, J.J. *et al., J. Mater. Chem.* **2012,** *22*(20), 10235-10248.

Radiation Hardness

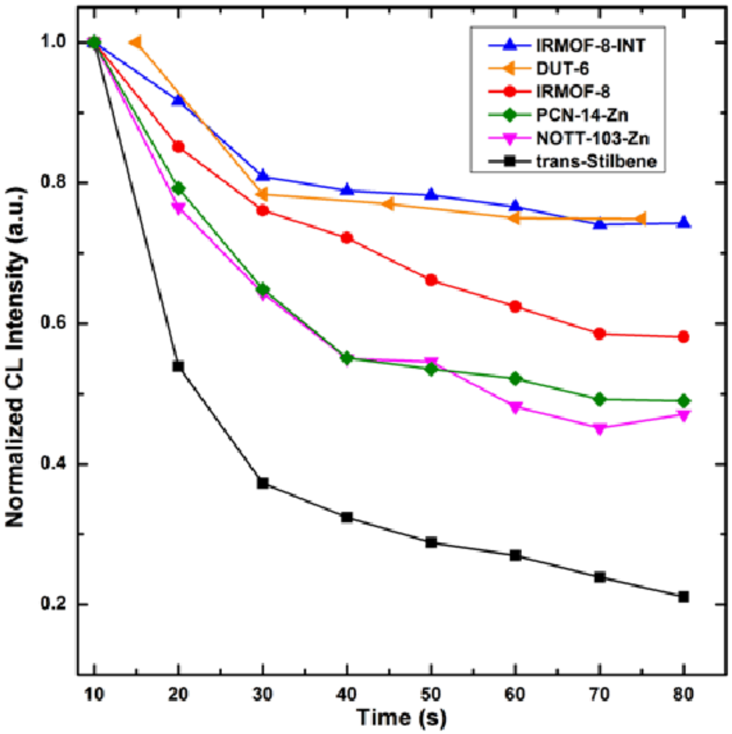
MOFs exhibit resistance to radiation damage more typical of amorphous materials than crystalline organic scintillators !





Steady-State CL Spectra taken at 10 s time intervals

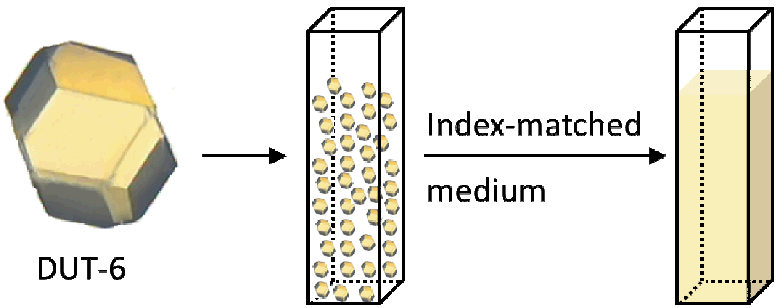
5 kV, 0.9 nA

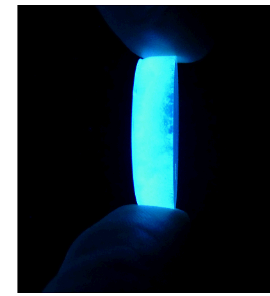


MOF's rate of intensity decay lower

Total Intensity loss only 25% - 60 % that of *trans*-stilbene

Index-Matched Bulk Scintillator



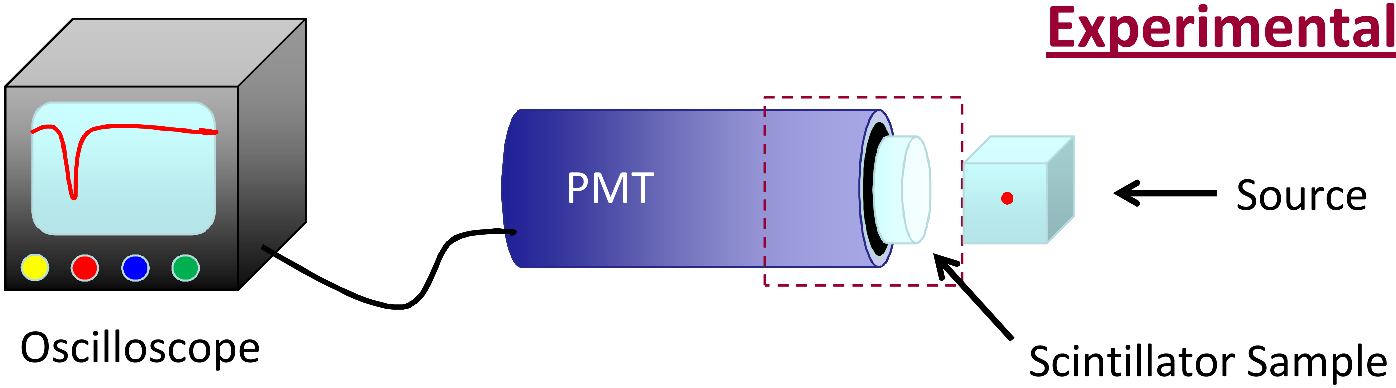


Fluid	RI
Air	1.0003
Water	1.333
Hexane	1.375
Chloroform	1.446
Benzene	1.501
Carbon disulfide	1.74
MOF Scintillator DUT-6	1.70

Polymer	RI
Polymethylmethacrylate	1.489
Polycyanoacrylate	1.48
Polycarbonate	1.584
Polystyrene (PS)	1.60
Polydichlorostyrene	1.624
Poly (pentabromophenyl methacrylate)	1.71
Polytrithiocarbonate	1.78

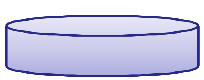
Proof of Concept: MOF PSD

Experimental Setup



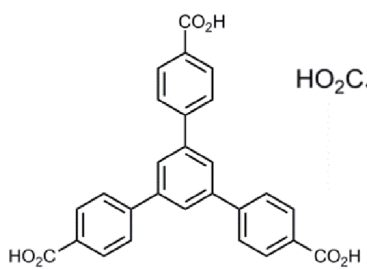
MOF Bulk Scintillator

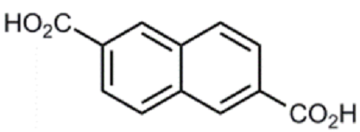
- DUT-6: BTB, NDC
- Polystyrene matrix (55% v)
- Right circular cylinder *ca.* 1” diam. X 5 mm thick



Radioactive Sources

- ^{60}Co (γ): 6.96 μCi
- AmBe (γ + n^0): 30.2 mCi

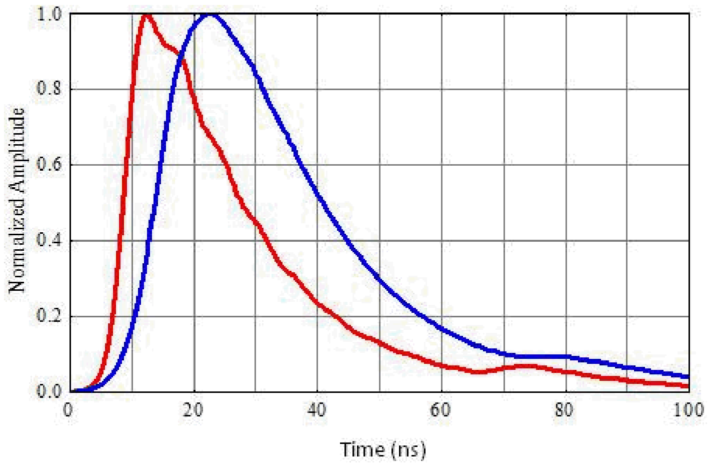




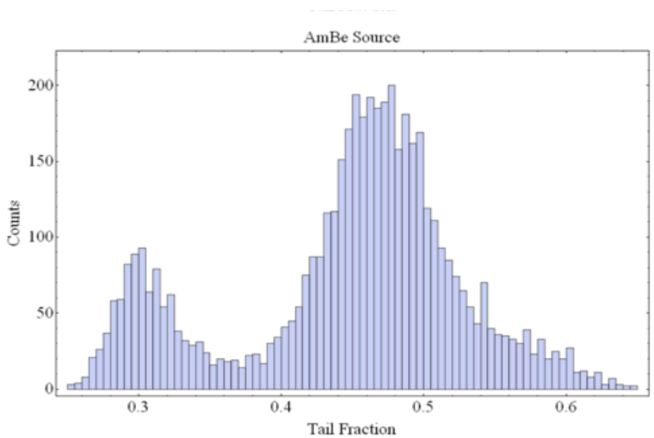
Hardware

- 12-bit LeCroy HRO 66Zi
  600 MHz max bandwidth
- 1.13’’ diam. PMT
  Fused Silica(ET Enterprises 9124QB)
- Oscilloscope used for pulse digitization and post processing

Pulse-Shape Discrimination



Averaged Pulse shapes (1000 pulses)
Red: AmBe (γ + n^0); **Blue**: ^{60}Co (γ)



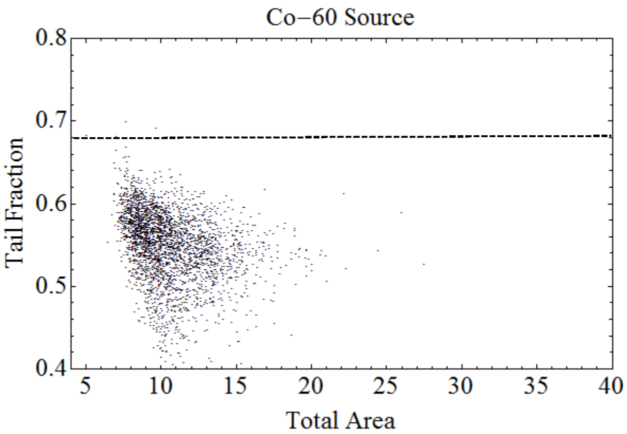
AmBe neutrons cause pulse rise-times 2X as fast as that of γ-rays

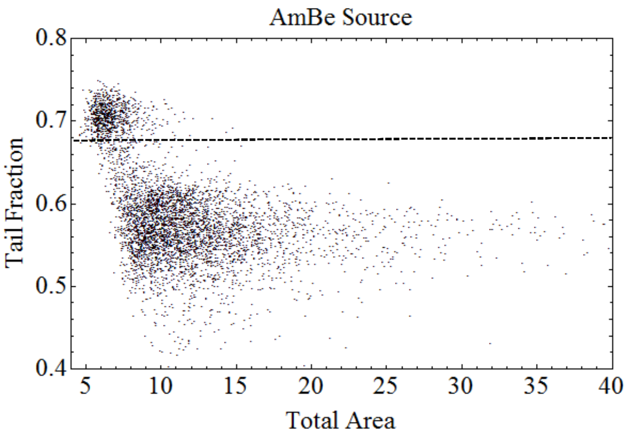
Exponential decay

< 20 ns time constant

Efficient rise-time discrimination @ high rates

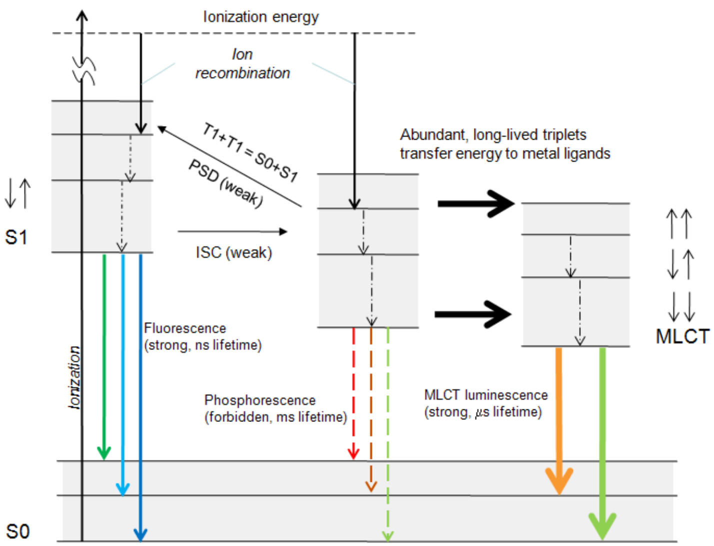
PSD FOM = 1.3





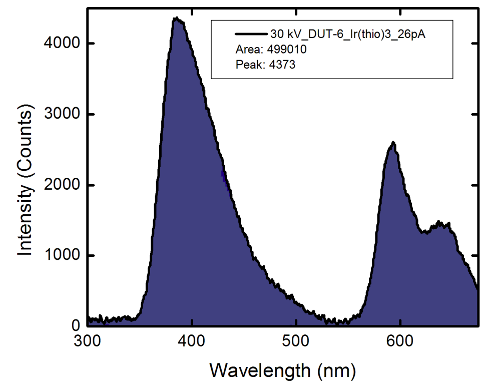
Total Area vs. Tail Fraction

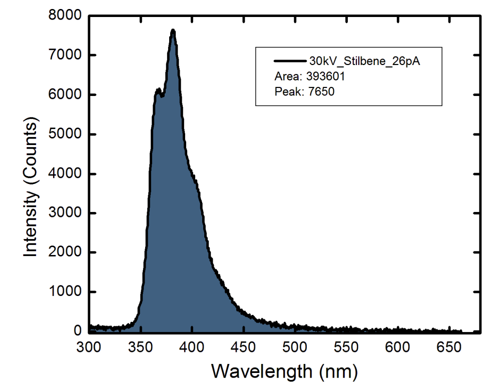
Spectral-Shape Discrimination



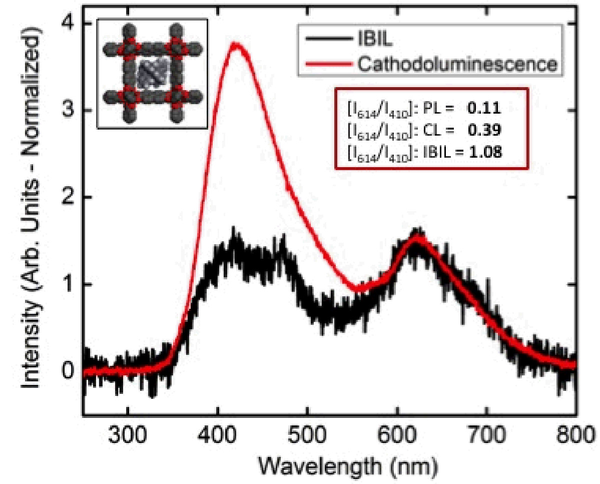
Tunable energy levels of MOF and Ir complex T_n

Ir fluor infiltrated DUT-6

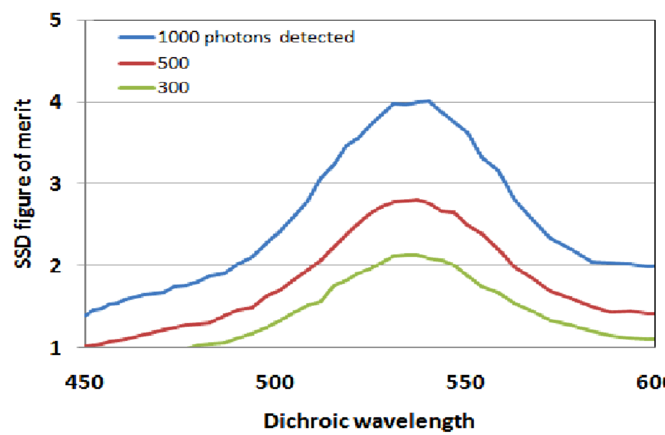


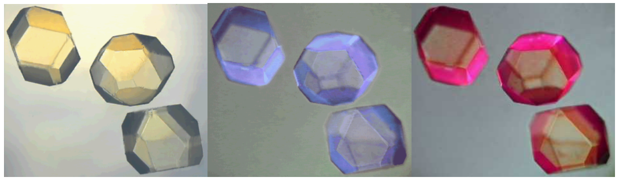


Ir fluor infiltrated IRMOF-8



Optimization of dichroic wavelength



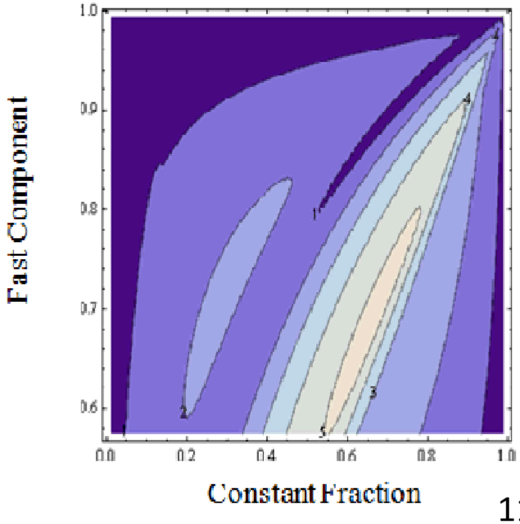


Conclusions

- Tunable luminescence decay times
- Bright Scintillators
- Tunable H:C ratio
- Demonstrated PSD and SSD
- Gamma rejection (PSD): $1x10^{-3}$
- Gamma-neutron FOM: 4 (SSD) ; 1.3 (PSD)
- Low refractive index, cubic crystals amenable to consolidation

Future Work

- Improve MOF / polymer index match
- Optimize MOF / Triplet Harvester interaction
- PAQS model for Pulse-Shape Engineering
- Increase H:C ratio
- Increase R_γ and FOM



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