

# Toward Predictive Design of Water-Based Liquid Scintillators for Hybrid Cherenkov/Scintillation Neutrino Detectors

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# There's no ultimate scintillator



## Two major strategies in scintillation research

The Edisonian approach of trial and error

The accidental discovery



*cook and look* Example: Nal:Tl *serendipity* Example: BGO

## Symphony No. 5 in C Minor

First Movement





When choosing 8 notes out of 12 tones where order matters and with repetitions...

Number of permutations:  $12^8 = 429981696$ If playing the motif takes 8 seconds...

...trying all permutations takes **112 years** of playing 24/7 365 days

Combinatorial approach to material discovery is prohibitively inefficient!



### The Edisonian approach of trial and error



cook and look

### The accidental discovery



serendipity

#### The rational design



#### enlightenment





Fig. 2.4 Ultraviolet spectra of polyenes. Replotted with data from [3]

### Molecular physics

Electronic/vibrational states Electronic transitions Quantum efficiency Photoluminescence





<2 nm

### Microphysics

Resonant energy transfer D-A interactions Molecular diffusion Rotation Solvent effects



2 nm – 15 nm

### Macrophysics

Light scattering Radiative transport Trace impurity absorption



## Challenges

sion is therefore increased. There appears to be no simple and reliable method to precisely quantify and correct for these concentration effects. It is best to avoid these problems by working with dilute solutions.

- Most of photophysical data have been collected in so called "neat solutions"
- There are no reliable models how to derive photophysical properties of high concentration solutions from diluted solution properties
- Trying to define photophysical properties in a mechanistic way may fail due to emergent effects. Examples: stilbene QE in solution
- Impurities may dominate the system response, very hard to deal with



#### The Periodic Table of the Elements





\* The lanthanoids (atomic numbers 58-71) and the actinoids (atomic numbers 90-103) have been omitted

The relative atomic masses of copper and chlorine have not been rounded to the nearest whole number

# **Properties = Composition + Structure**























 $OD = \log_{10} \frac{I_0}{I}$ 





## Why ultrafast spectroscopy?

Accessible only through ultrafast techniques:

- Transient absorption (pump & probe experiments)
- Ultrafast luminescence (time & wavelength resolved)







## Why laser spectroscopy?







Laser spectroscopy





The ultimate grand piano



INPE

Ultrafast photoluminescence setup coming soon!

