Advancing Phosphor Science:
Targeting high-efficiency phosphors *via* informatics

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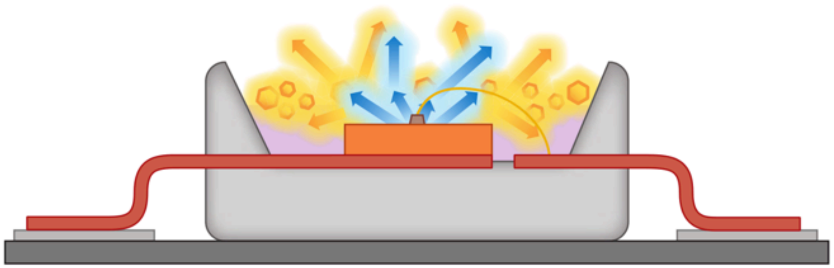
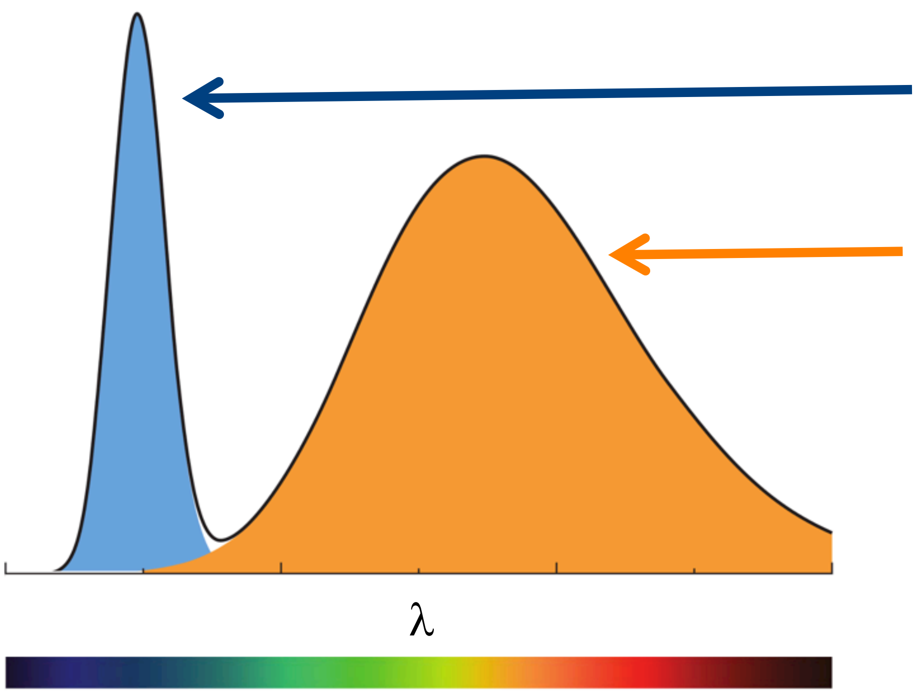
Phosphor converted solid-state white lighting

LED + yellow phosphor



Emission characteristics



White LEDs use a blue (450 nm) or near-UV (405 nm) that is partially converted by a phosphor.

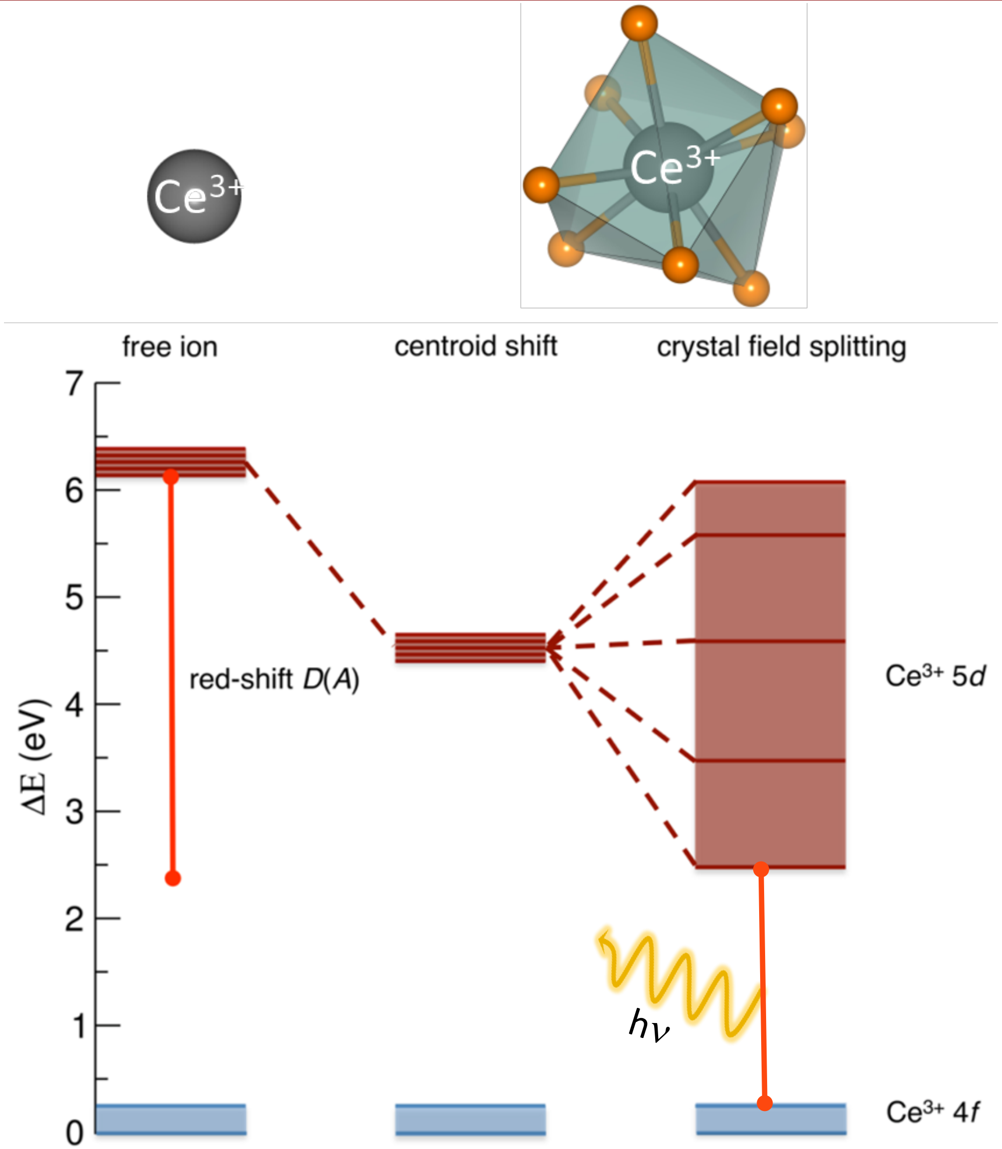
The combination of the LED emission and phosphor emission appear as white light.

LED + Phosphor
Radiation from LED
(absorbed by phosphor)

Radiation from phosphor down-conversion
(emission from phosphor)

George, Denault, and Seshadri *Annu. Rev. Mater. Sci*, **2013**, *43*, 2.1:2.21

Mechanism of phosphor emission in white LEDs



Phosphors consist of two components: activator ion (luminescent center) and a host lattice

Emitted light can be tuned to desired wavelength by changing the CFS of the activator ion

George, Denault, and Seshadri *Annu. Rev. Mater. Sci*, **2013**, *43,* 2.1:2.21

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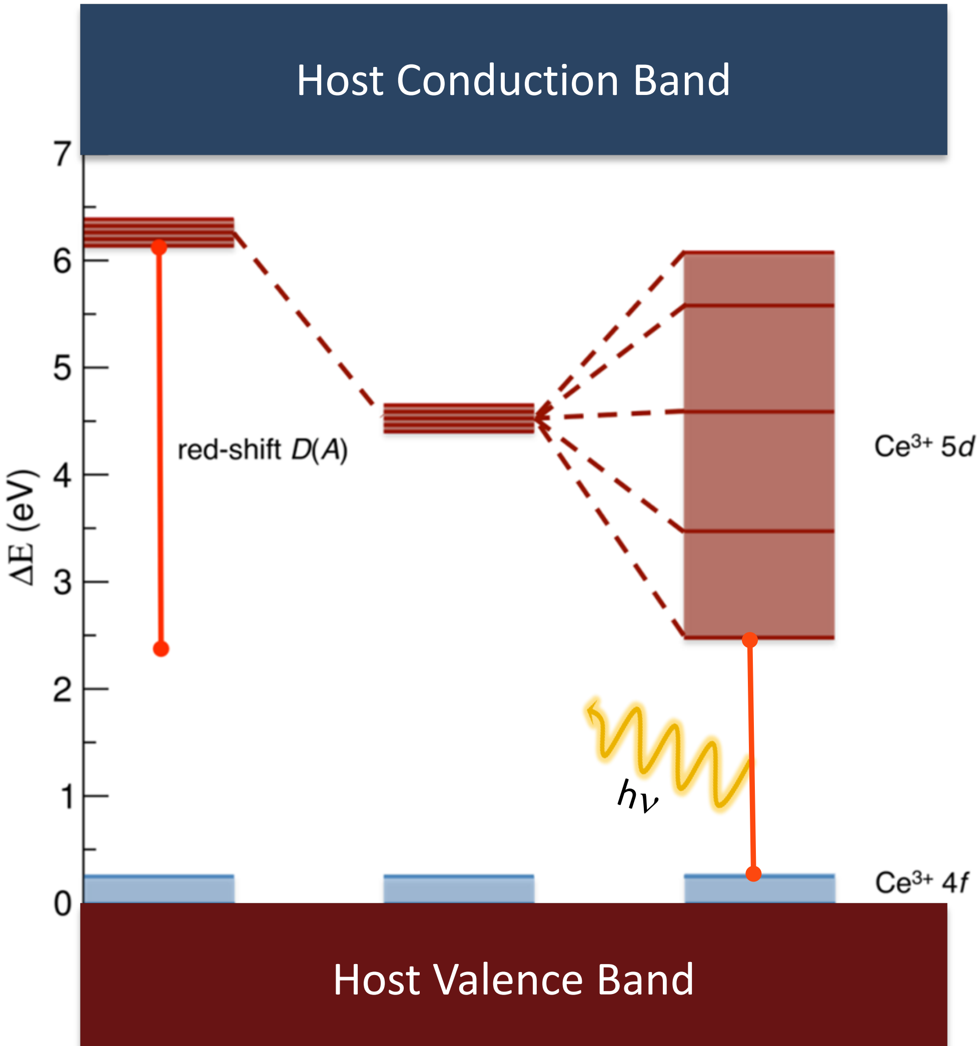


Phosphors consist of two components: activator ion (luminescent center) and a host lattice

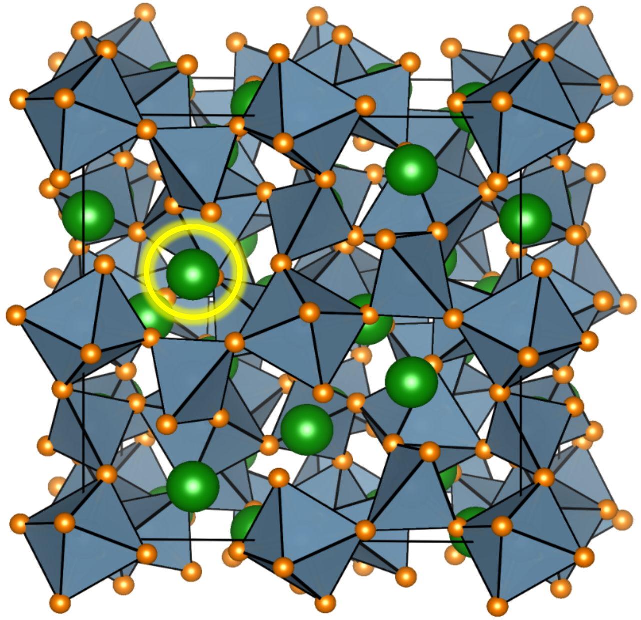
Emitted light can be tuned to desired wavelength by changing the CFS of the activator ion

The photophysics occurs in the band gap

- Need wide band-gap materials that can accommodate the *RE*

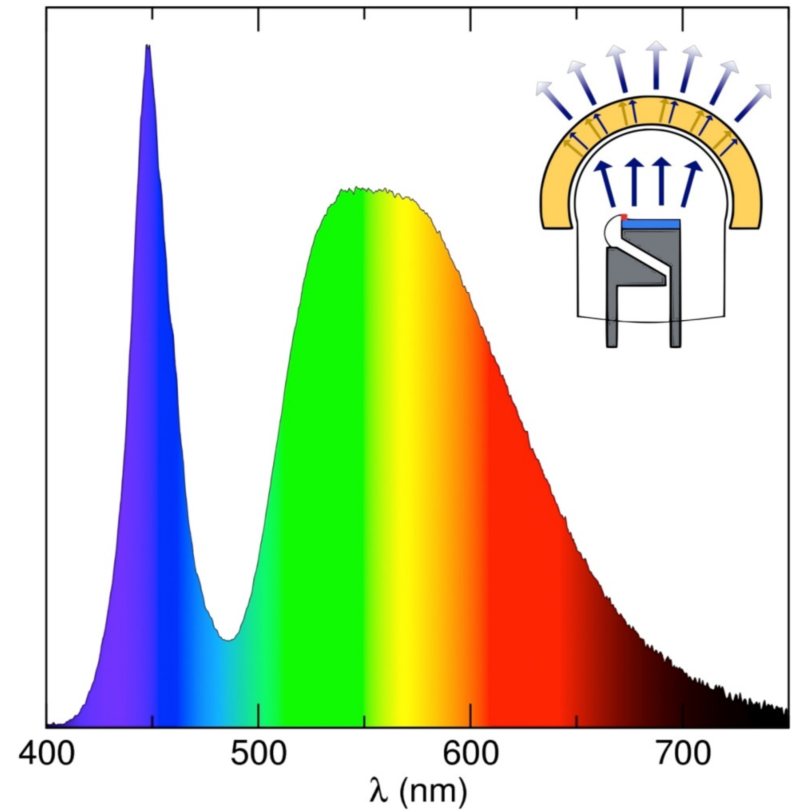
Cerium-substituted YAG: The prototypical phosphor

$(Y_{2.97}Ce_{0.03})Al_5O_{12}$

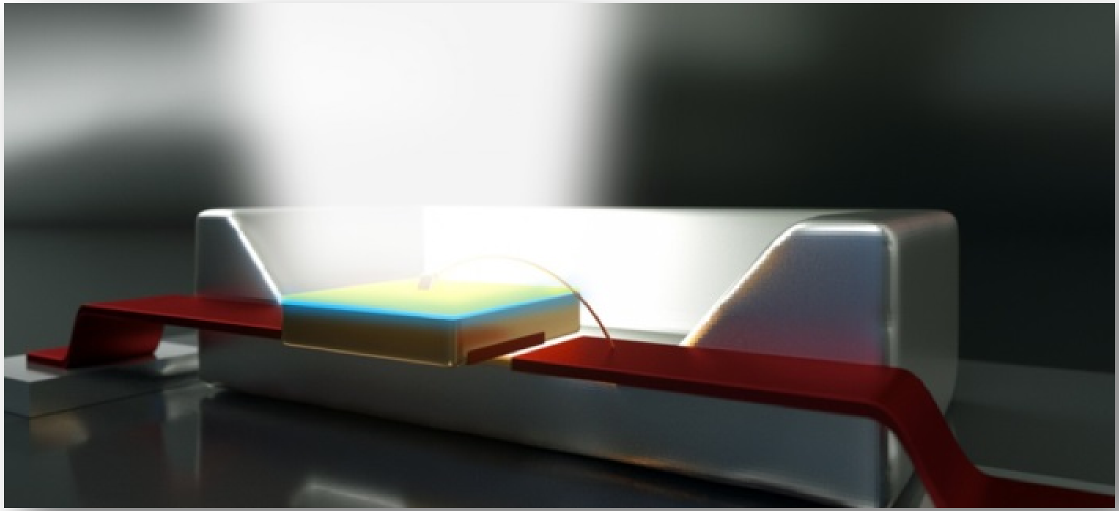


Cerium-substituted yttrium aluminum garnet (YAG:Ce^{3+}) is a widely used phosphor because of its high photoluminescent quantum yield (PLQY= 80-95%)

Absorbs blue and then down converts to a yellow emission



The need for new phosphors

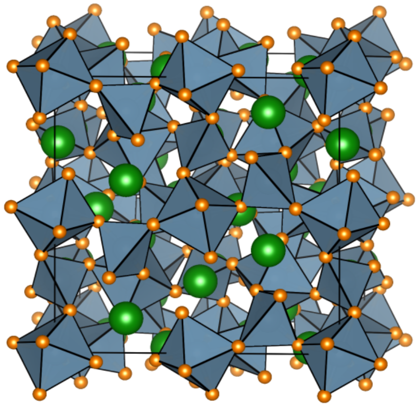


A better approach to develop new, efficient inorganic phosphors

Develop phosphors that have enhanced thermal quenching properties for high-power LED and laser based lighting

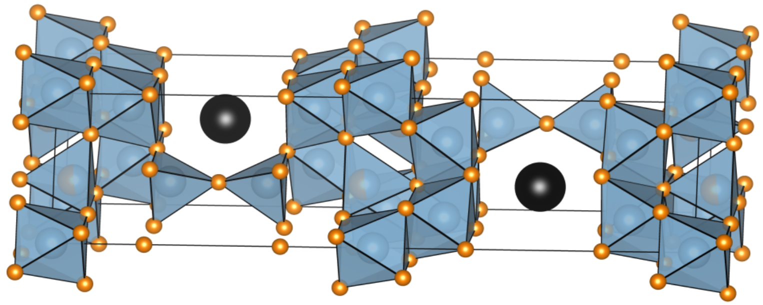
A more efficient method to identify new phosphor hosts

$Y_3Al_5O_{12}:Ce^{3+}$



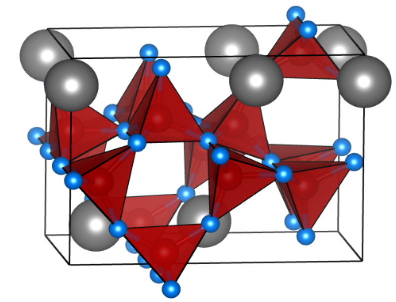
Yellow Emission
90 % Efficient
(*Chem. Mater.* **2009** *21*, 316)

$BaMgAl_{10}O_{17}:Eu^{2+}$



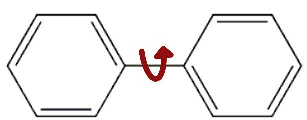
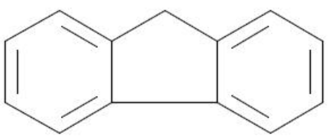
Blue Emission
92 % Efficient
(*Chem. Mater.* **2002** *14*, 5045)

$Sr_2Si_5N_8:Eu^{2+}$



Orange/Red Emission
80% Efficient
(Appl. Phys. Lett. **2011** *99*, 241106)

Highly rigid structures improve photoluminescence efficiency
This is well known in molecular chemistry …

biphenyl  *vs.*  fluorene

How do we measure structural rigidity in a solid?

Calculating Debye temperature from the elastic constants

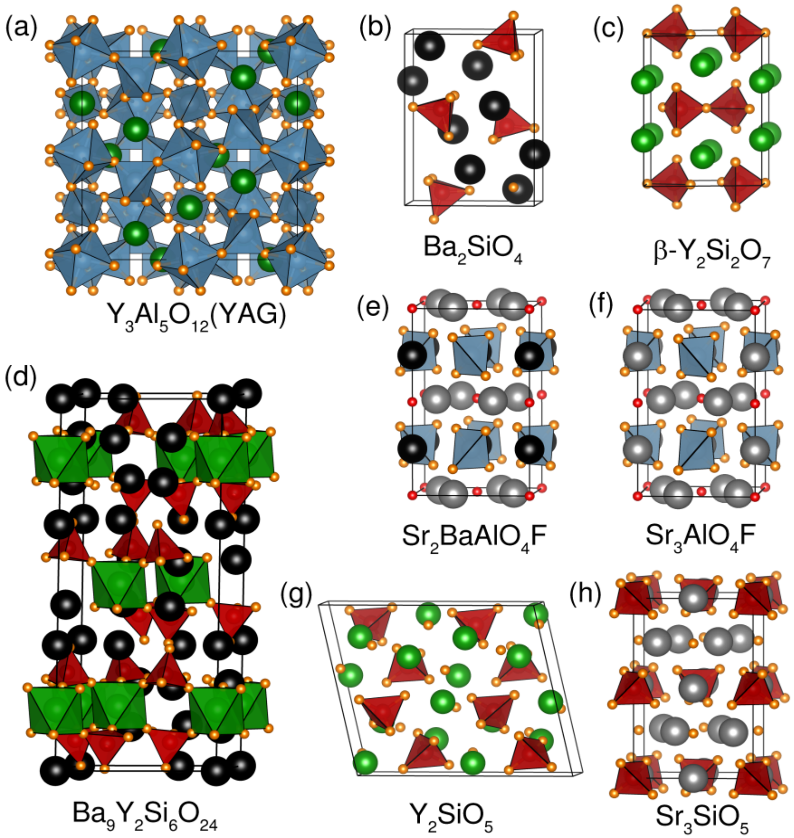
$$\Theta_D = \frac{\hbar}{k_B}[6\pi^2 V^{1/2} n]^{1/3}\sqrt{\frac{B_H}{M}}f(\sigma)$$

$$f(\sigma) = \left\{3\left[2\left(\frac{2}{3}\cdot\frac{1+\sigma}{1-2\sigma}\right)^{\frac{3}{2}} + \left(\frac{1}{3}\cdot\frac{1+\sigma}{1-\sigma}\right)^{\frac{3}{2}}\right]^{-1}\right\}^{\frac{1}{3}}$$

V = unit cell volume
n = number of atoms
B_H = bulk modulus
M = molar mass
σ = Poisson's ratio
$f(\sigma)$ = function of Poisson's ratio

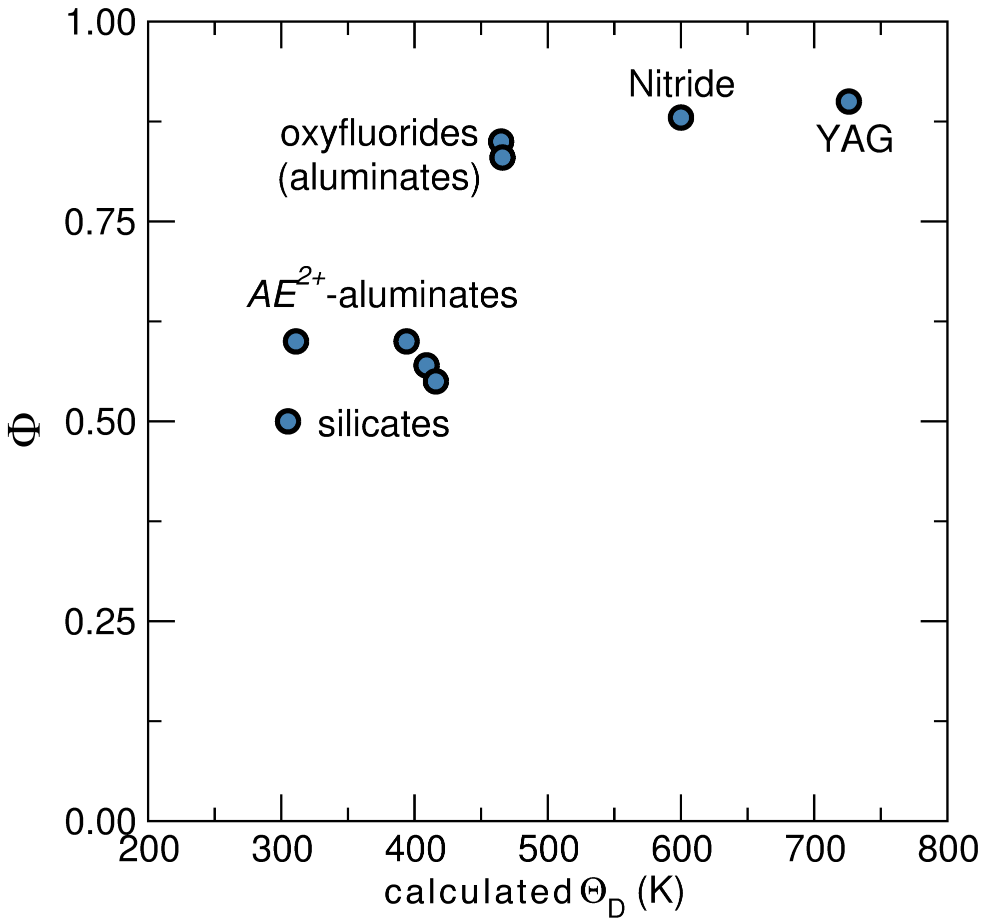
B_H and Poisson's ratio can be calculated from stress-strain relationships determined by first-principles (VASP)

Examples of phosphor hosts screened



Brgoch, DenBaars, and Seshadri *J. Phys. Chem. C* **2013**, *117*, 17955-17959.

Quantum yield of Ce^{3+} phosphors follow Debye temperature



Quantum yield (Φ) increases with Debye temperature

Aluminates tend to have the highest Debye temperature and largest quantum yield of the compounds examined so far

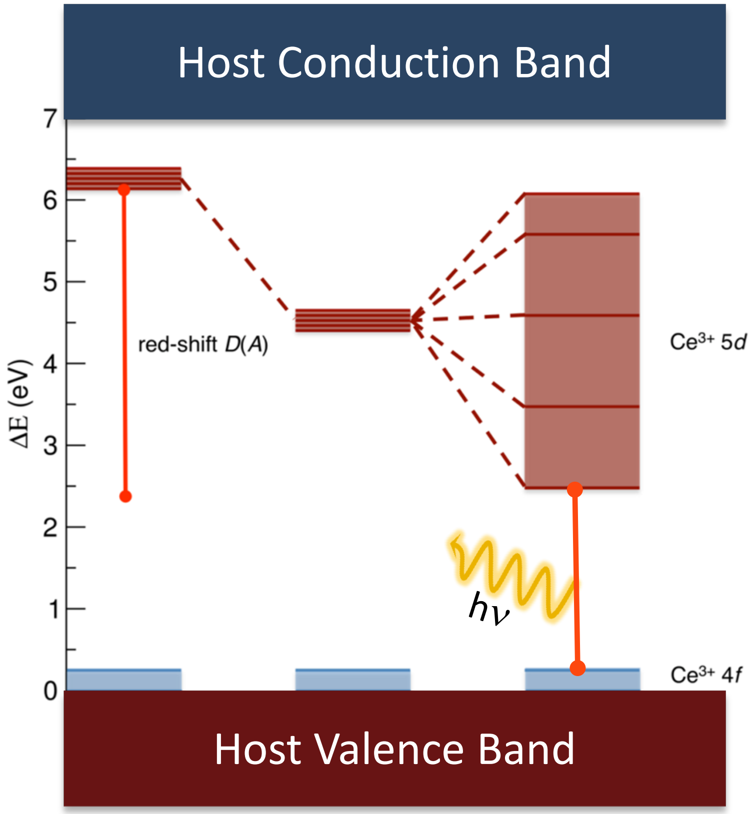
Brgoch, DenBaars, and Seshadri *J. Phys. Chem. C* **2013**, *117*, 17955-17959.

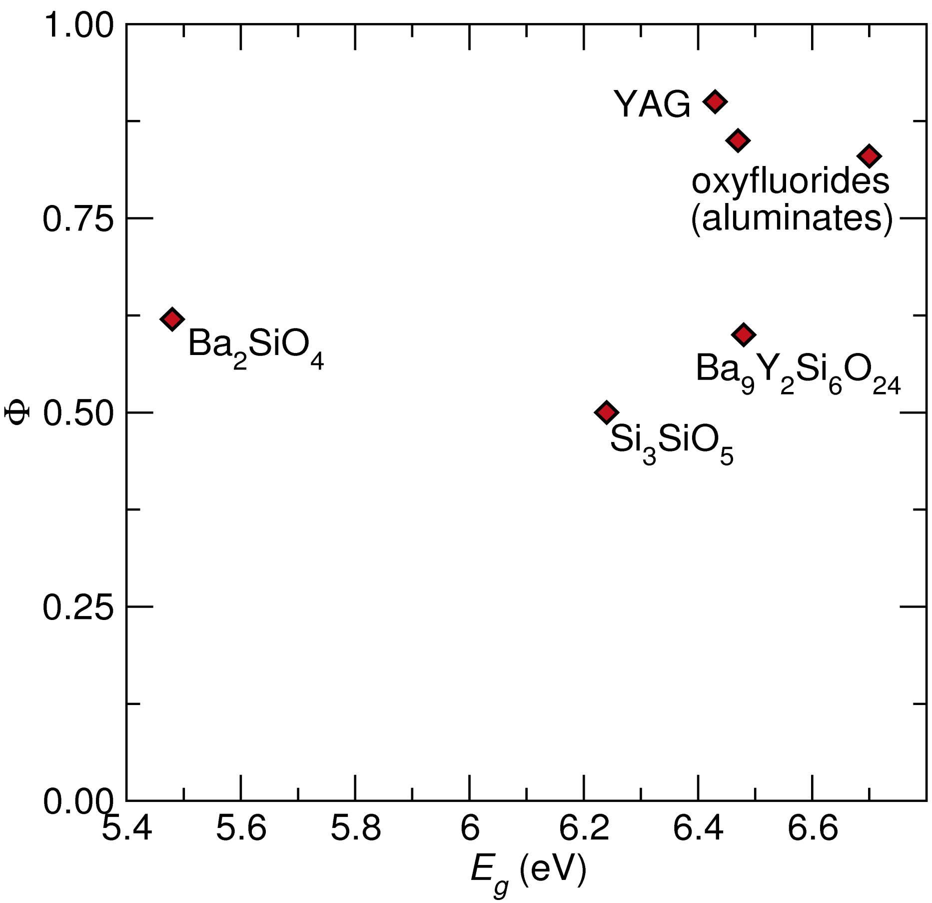
Phosphor hosts need to have a wide band-gap for the *RE* orbitals

A small gap can lead to emission quenching due to thermal population of the conduction band

To use this approach as a screening tool compound must have a wide band gap

The band gap is accurately calculated using hybrid functional calculations (HSE06)





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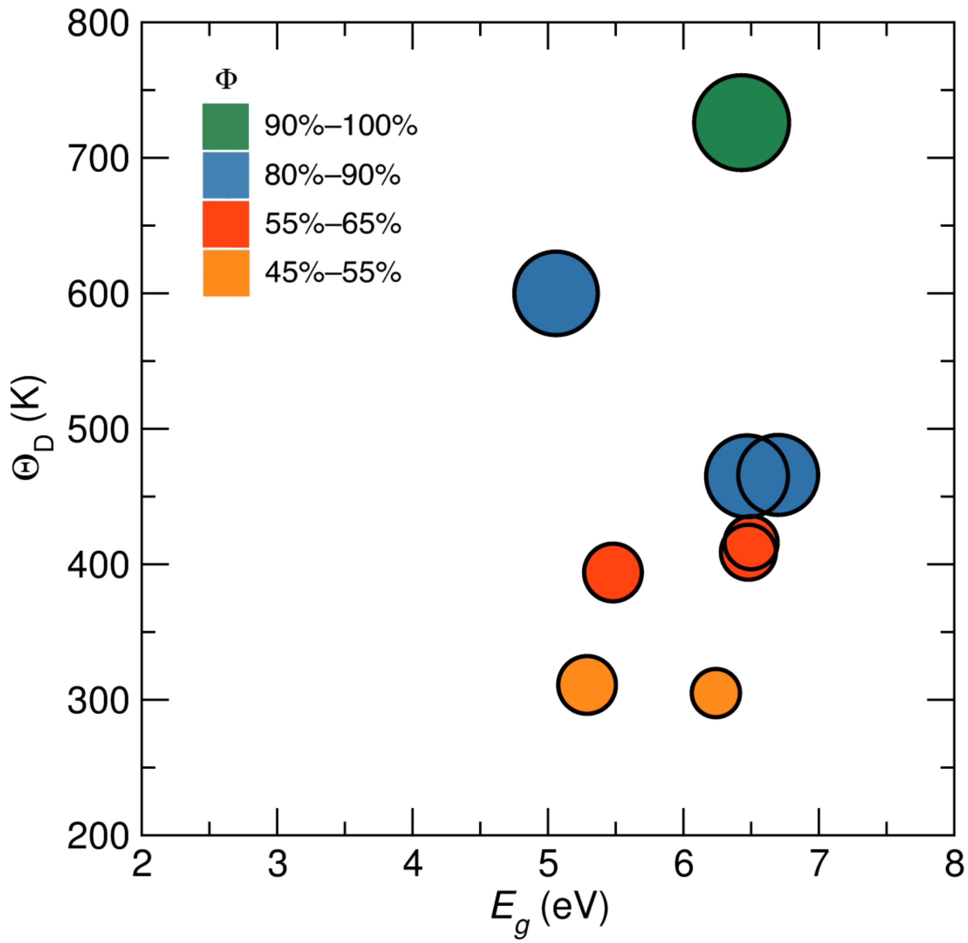
Sorting diagram for efficient (Ce^{3+}) phosphor hosts

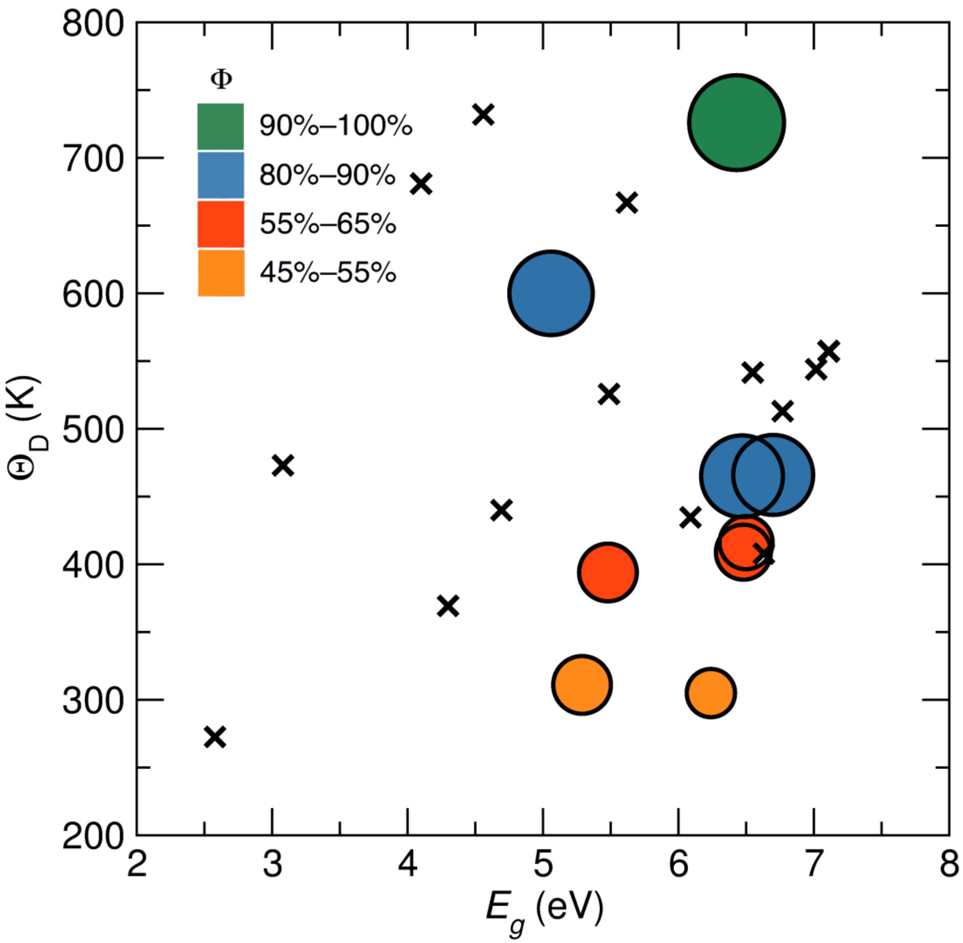


Plotting Debye temperature against band-gap can be used to identify compounds that have the optimal properties

- The most efficient materials fall in the top-right corner

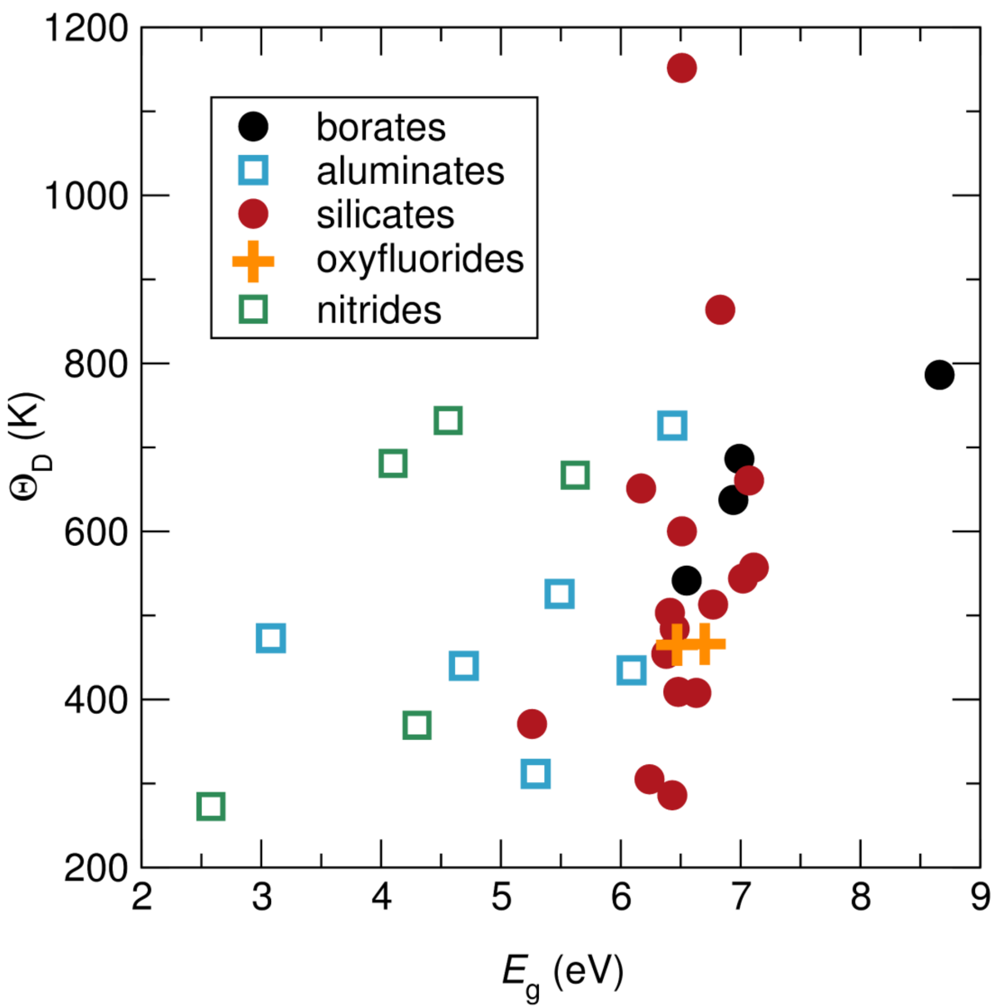
Brgoch, DenBaars, and Seshadri *J. Phys. Chem. C* **2013**, *117*, 17955-17959.

Screening for efficient phosphor hosts



Searching structural through crystal structure databases, *e.g.*, the ICSD, indicates the potential targets for synthetic consideration

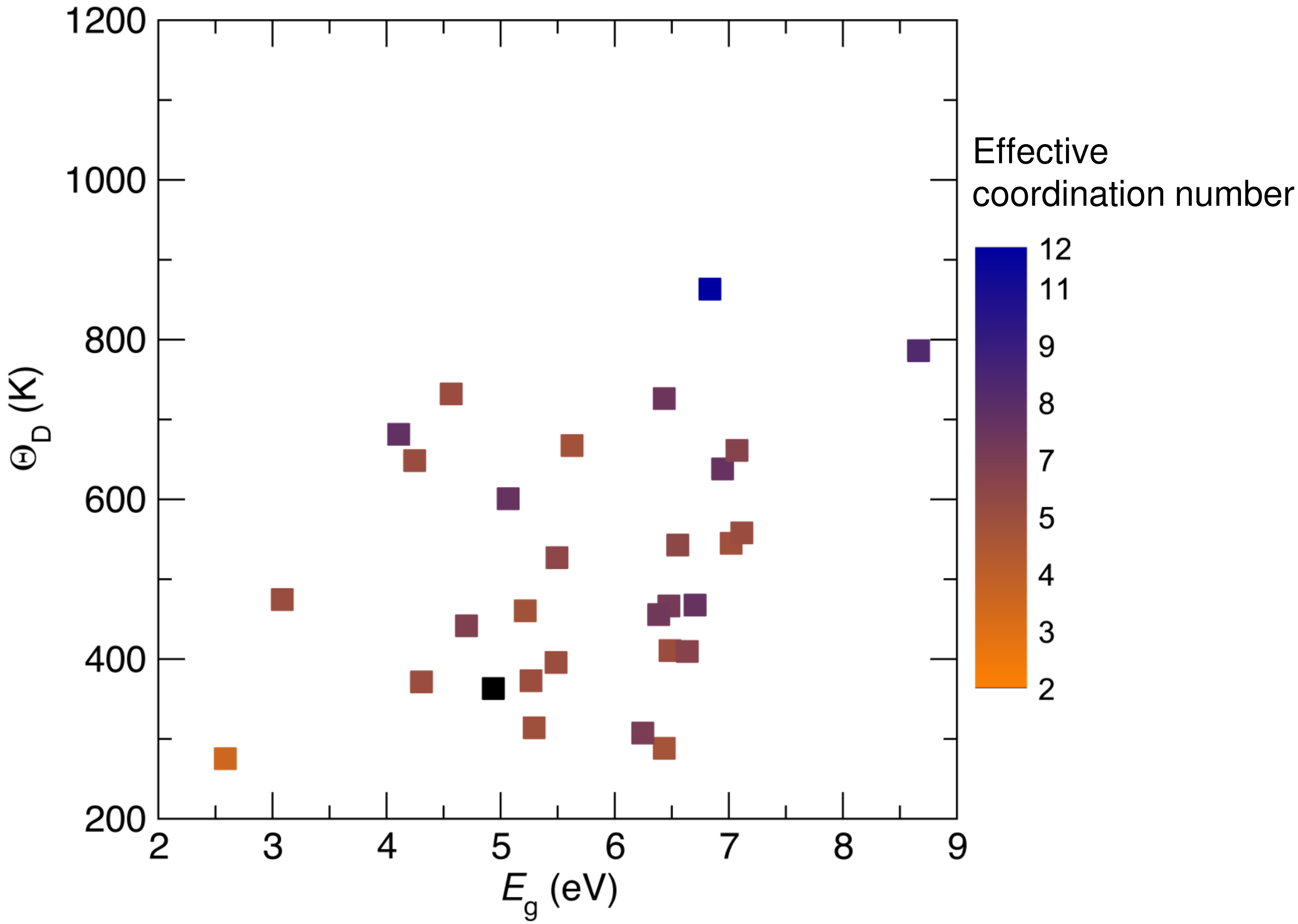
Learning from large data-sets – Compositional information



Examining metadata provides an indication of where to focus the future search

- Oxides are still a great place to focus – in particular borates

Learning from large data-sets – Coordination environments



Examining metadata provides an indication of where to focus the future search

- Oxides are still a great place to focus – in particular borates
- Higher coordination environments appear to be favorable in efficient phosphors

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