Materials Seminar

Prof. Ram Seshadri

Univ. of California, Santa Barbara

Materials Department &
Dept. of Chemistry & Biochemistry

DFT-based proxies for materials screening: Examples of phosphor hosts and magnetocalorics

My talk will address phosphors that play a key role in the now almost-mature solid-state white-lighting technologies based on combining a III-nitride-based near-UV or blue solid-state light source with down-conversion to longer wavelengths. Almost all widely used phosphors comprise a crystalline oxide, nitride, or oxynitride host that is appropriately doped with either Ce^{3+} or Eu^{2+}. Optical excitation into these states and concomitant reemission can be tuned into the appropriate regions of the visible spectrum by the crystal these ions are hosted in. Experimental studies of some of the best phosphor materials, employing state-of-the-art structural tools, have yielded guidelines for what are desirable structural features. We find that a useful sorting diagram for efficient hosts with high quantum yield has the band gap of the host – readily calculated with high reliability using hybrid functionals in DFT – as one of the axes, and the calculated Debye temperature as the other axis.

In the second part, I describe a new effort to seek out exciting new room-temperature magnetocaloric materials. The material property of interest in finding candidate magnetocaloric materials is their gravimetric entropy change upon application of a magnetic field under isothermal conditions. We have proposed a simple computational proxy based on carrying out non-magnetic and magnetic density functional theory calculations on magnetic materials. This proxy, which we refer to as the magnetic deformation Σ_M, is a measure of how much the unit cell deforms when comparing the relaxed structures with and without the inclusion of spin polarization. Σ_M appears to correlate very well with experimentally measured magnetic entropy change values.

Thursday, Sept. 21, 12:15 pm   Rm 1315 Chemistry