MRSEC SEMINAR SERIES

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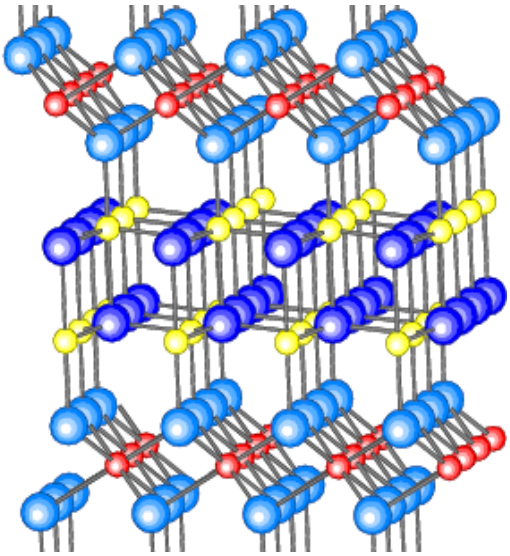
2:00PM Ryan 4003

Transparent conductors:

From basic principles to controllable properties

The unique combination of two mutually exclusive properties – optical transparency and electrical conductivity – is known to be a prerogative of only a few oxides of post-transition metals, In_2O_3, ZnO, CdO and SnO_2. Rapid development of technologies for which transparent conducting oxide (TCO) is a vital component stimulate further research aimed at (i) broadening the range of the electronic and optical properties of application-specific TCO in a controllable way; and (ii) designing novel materials as a viable, inexpensive alternative to conventional TCOs.



Here, we employ first-principles density-functional approach to investigate the structural, electronic and optical properties of several classes of transparent conductors including conventional single-cation and multi-component main-group metal oxides as well as non-oxide materials, and to determine the role of the crystal structure, chemical composition and carrier generation in the resulting properties.

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