Defects and transport in functional materials

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Course description:

Many functional materials properties involve charge transport by ions or electrons in the form of defects. The thermodynamics and transport mechanisms of such defects are central in order to understand structure-composition-properties relationships and develop new materials and doping strategies. The lecture will introduce defect chemistry and transport mechanisms in light of the applications of various materials. Experimental characterization of defects thermodynamics and transport will be discussed, with special attention to diffusivity and conductivity, elevated temperatures, atmosphere control, sample geometries (including thin films), and parasitics. Atomistic ab initio and other computational modeling of defects and transport will also be covered.

Syllabus of the lecture subjects (enlisted):

1. Introduction and overview of functional materials
2. Structure and defects
3. Defect chemistry; theory and measurements
4. Diffusion mechanisms; theory and measurements
5. Electronic and ionic conductivity
6. High temperatures and controlled temperatures
7. Sample geometries and parasitics
8. Computational methods
9. Review and conclusions

TERMINY ZAJĘĆ			
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