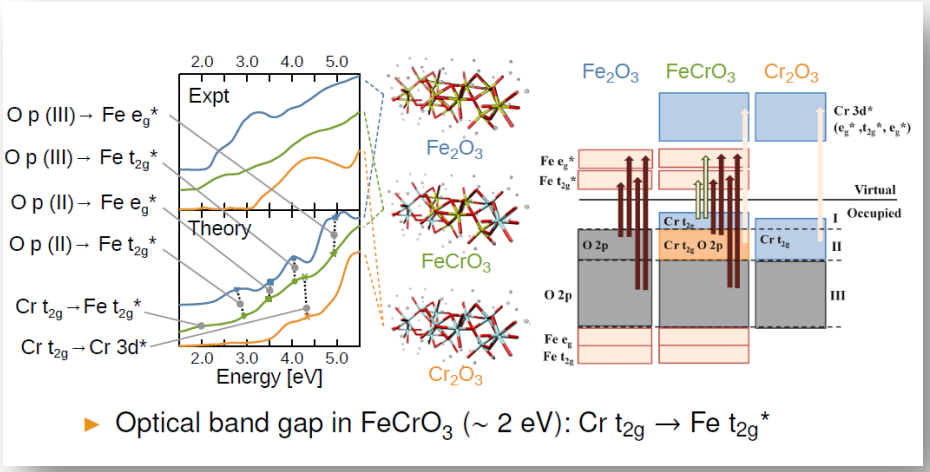
Optical Absorption in α-$(Fe_{1-x}Cr_x)_2O_3$ Solid-Solution Thin Films



► Optical band gap in $FeCrO_3$ (~ 2 eV): Cr t_{2g} → Fe t_{2g}*

Experimental and calculated real-time TDDFT optical absorption spectra and schematics of the optical transition types. The dark arrows are transitions to the unoccupied Fe t2g* and eg* states. The light arrows are the transitions to the unoccupied Cr 3d states. The light arrows with dark outlines are transitions from occupied top Cr t2g to unoccupied Fe t2g* and eg* states. The occupied states are separated as indicated by black dashed lines into three regions: I, II, and III. Note that the widths of regions I and II are not to scale.

Reference: Y. Wang, K. Lopata, S.A. Chambers, N. Govind, P. V. Sushko, J. Phys. Chem. C, 117 (48), 25504-25512 (2013), Publication Date (Web): November 8, 2013

Work was performed at Pacific Northwest National Laboratory

Scientific achievement

Theoretical and experimental study of the optical response of α-$(Fe_{1-x}Cr_x)_2O_3$ solid solutions for visible light photo-catalysis

Significance and Impact

First detailed study of the optical response of this material. Highlights new computational approach for dense and large numbers of optical transitions.

Research Details

- Used recently developed real-time (RT) TDDFT in NWChem in conjunction with the embedded cluster method to shed light on closely spaced optical transitions.
- Studied the optical spectra of pure α-Fe_2O_3, α-Cr_2O_3 and α-$(Fe_{0.5}Cr_{0.5})_2O_3$ and assigned the character of the main optical absorption bands for photon energies up to 5.5 eV. Calculations demonstrated that Fe-Cr mixing gives rise to new spin-allowed optical transitions.