PRB: Orbital Polarization

Origin of the orbital polarization of Co2+ in La2CoTiO6 and (LaCoO3)1+(LaTiO3)1: A DFT+U and DFMT study

Points (Resolved)

- Ligands cause the crystal field to split:
  - Large split (aka Strong Field Ligands) implies low spin and vice versa
- Splitting is also determined by the oxidation state of the ligand

Questions

Ligand/Crystal Field Theory

- What is meant by the 'Strength' of a ligand?
- What are the main assumptions of Crystal field theory
- How is CFT different from Ligand Field Theory
- Why is the Spectrochemical Series backwards to what is said by the Crystal Field Theory
- Jahn Teller Effect
- Octahedral Tilting and Glazer Notation (Clarification)
  - What causes it?
  - How to show it using Vesta/VMD?
- Electron-Lattice coupling
- Superexhcange interactions
- Goodenough-Kanamori Rules
- Superlattice

DFT

Meeting 3

Meeting 2

Meeting 1

Agenda for Meeting 2:

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- Discuss Crystal Field Theory literature
    https://www.youtube.com/watch?v=V1WSesBeURw
    Figgis: Ligand Field Theory and Its Applications
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Terminology

What are:

- Spectrochemical Series:
- Goldschmidt's Tolerance Factor: predicts the stability of perovskites.