

Prezentare coordonator

1. Conducator de doctorat: Avram Nicolae

2. Scurta descriere a domeniului de cercetare "Modelare si simulare in spectroscopie".

In cadrul acestui domeniu de cercetare se desfasoara activitati vizand:

- Modelarea si simularea de proprietăți structurale, electronice, optice si spectrale ale unor materiale de interes tehnic (cristale, sticle, ceramici, nanomateriale), pure sau dopate cu ioni ai metalelor de tranziție;
- Modelarea parametrilor câmpului cristalin si ai Hamiltonianului de spin si simularea schemelor nivelelor energetice si a tranzițiilor dintre ele pentru ionii metalelor de tranziție;
- Simularea proprietăților spectrale ale unor materiale optice (oxizi, fluoruri) dopate, folosind primul principiu;
- Extragerea parametrilor câmpului cristalin pe baza unor metode *ab initio* CASSCF si multireferințiale;

3. Tema de cercetare pentru studiul doctoral si bibliografia aferenta:

"Obtinerea de noi informatii despre proprietatile spectrale ale spinelilor normali (Mg, Zn)Al₂O₄ dopati cu Cr³⁺/ Co²⁺ folosind metode multireferintale".

Bibliografie minimala:

1. N.M.Avram and M.G.Brik (Eds), *Optical Properties of 3d-Ions in Crystals.Spectroscopy and Crystal Field Analysis*, Tsinghua University Press, Beijing and Springer-Verlag, Berlin,Heidelberg, 2013, pp. 29-94.

2. Mihail Atanasov,Emiliana-Laura Andreici Eftimie, Nicolae M. Avram, Mikhail G. Brik and Frank Neese, "*First-principles study of optical absorbtion energie, ligand field and spin-Hamiltonian parameters of Cr³⁺ ions in emerald*", Inorg. Chem., **61**, 178-192 (2022)

4. Teme propuse pentru proba de specialitate la admitere si bibliografia aferenta (de regula 5 subiecte):

- Simetria cristalelor, grupuri de simetrie;
- Spectrele atomilor liberi cu mai multi electroni;
- Spectrele ionilor metalelor de tranzitie dopati in cristale;
- Notiuni de baza DFT;
- Metode ab initio alicate la cristale dopate;

Bibliografie

1. N. M. Avram, C. N. Avram, *Nivele energetice ale ionilor in cristale*, Ed. Mirton, Timisoara,

1 991.

2. Brik M. G., Ma C-G. *Theoretical Spectroscopy of Transition Metal and Rare Earth Ions: From Free State to Crystal Field*. Singapore: Jenny Stanford Publishing, 2020.

3. Henderson B, Bartram R H. *Crystal-field Engineering of Solid-State Laser Material*, Cambridge University Press, 2000.

1. **PhD supervisor:** Avram Nicolae

2. **Brief description of the research field** "Modeling and simulation in spectroscopy".

Within this field of research, activities are carried out aiming at:

-Modeling and simulation of structural, electronic, optical and spectral properties of materials of technical interest (crystals, glasses, ceramics, nanomaterials), undoped or ion-doped transition metals;

- Modeling the parameters of the crystalline field and the spin Hamiltonian and simulating the schemes of energy levels and the transitions between them for the ions of transition metals;

- Simulation of the spectral properties of doped optical materials (oxides, fluorides), using the first principle;

-Extraction of the crystal field parameters based on ab initio CASSCF and multireference methods;

3. **Research topic for doctoral study and related bibliography:**

"Obtaining new information about the spectral properties of normal (Mg, Zn) Al₂O₄ spinel doped with Cr³⁺ / Co²⁺ using multi-reference methods."

References

1.N.M.Avram and M.G.Brik (Eds), *Optical Properties of 3d-Ions in Crystals.Spectroscopy and Crystal Field Analysis*, Tsinghua University Press, Beijing and Springer-Verlag, Berlin, Heidelberg, 2013, pp. 29-94.

2. Mihail Atanasov, Emiliana-Laura Andreici Eftimie, Nicolae M. Avram, Mikhail G. Brik and Frank Neese, "First-principles study of optical energy absorption, ligand field and spin-Hamiltonian parameters of Cr³⁺ ions in emerald", *Inorg. Chem.*, 61, 178-192 (2022)

4. **Proposed topics for the special exam at admission and the related bibliography (usually 5 subjects):**

-Symmetry of crystals, symmetry groups;

-Spectra of free atoms with many electrons;

- Spectra of transition metal ions doped in crystals;
- DFT basics;
- Ab initio methods for doped crystals;

References

2. N. M. Avram, C. N. Avram, *Energy levels of ions in crystals*, Ed. Mirton, Timisoara, 1991.
2. Brik M. G., Ma C-G. *Theoretical Spectroscopy of Transition Metal and Rare Earth Ions: From Free State to Crystal Field*. Singapore: Jenny Stanford Publishing, 2020.
3. Henderson B, Bartram R H. *Crystal-field Engineering of Solid-State Laser Materials*, Cambridge University Press, 2000.

Emeritus Professor Nicolae Avram