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TRADITIO ET EXCELLENTIA

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CS II Dr. Habil. Diana Benea

Competence domains:
Ab initio methods for describing the electronic structure of solids:

- Band structure calculations (KKR, LMTO) in solids
- Density functional theory
- Description of nonstoichiometric systems using the coherent potential approximation (CPA).
- Ab initio methods for description of the magnetic/spectroscopic properties of solids: magnetic Compton scattering, positron annihilation, X ray magnetic dichroism, XPS spectroscopy.

Research interests:
Currently, my research activity is related to the theoretical investigations of the electronic and magnetic properties of the solid-state compounds and spectroscopic properties of nanomaterials. Recent research topics are the following:

- New permanent magnets with lower cost and high performance of R-M-A/R-M type or MnBi/MnAl based alloys (R = Y and rare earth, M = transition metal 3d, A = metalloid, carbon or nitrogen). Theoretical calculations aim to predict new materials with low critical rare earth content, high anisotropy and high saturation magnetization in order to build rare-earth free permanent magnets with competitive performances.
- Half metal ferrimagnets with high spin polarization, presenting a Curie temperature above the room temperature which could be an ideal option for magnetoelectronic devices due to the very low energy losses. The electronic band structure calculations aim to predict the magnetic and electronic properties of half-metal compounds Heusler materials and to understanding the mechanism of half-metallicity and ferrimagnetism within these compounds, driven by the chemical composition and by exchange interactions responsible for the magnetic ordering.