

Title:

**New Advances in Theoretical Understanding of Rare-Earth Emission. Fundamentals for Applications by Rational Property Design.**

Acronym: NATURE

Project Code: PN-III-P4-PCE-2021-1881

Contract no.: 123/2022

Period: 2022-2024 (32 months)

Budget: 1.200.000,00

Funding: The Executive Agency for Higher Education, Research, Development and Innovation Funding (UEFISCDI), The Ministry of National Education, Romania

**Abstract:**

Logically and logistically, the project is built from objectives affirming, justified, the capacity of realistic simulation and rational predictions regarding the design of new scintillators based on lanthanides, usable in economical lighting devices, based on LED (Light-Emitting Diode) technology.

The project is built on the solid ground of pioneering achievements in the subtle and complicated field of lanthanide quantum chemistry. It is designed as a fundamental research approach, but the rational structure-properties relationships are of real interest, as guidelines for synthetic and instrumental experiments. Methodological aspects involve non-routine, first-principles calculations, insight into challenging new aspects of chemical bonding, and investment in models (Ligand Field models) with high heuristic power.