



DFT/DFPT Investigation of Functional Oxides and Nitrides: From Structural Stability to Electronic, Magnetic, and Thermoelectric Properties

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MARTES 16 DE JUNIO A LAS 12:00

**SALA DE SEMINARIOS DEL DPTO. DE FÍSICA DE MATERIALES
FACULTAD DE CIENCIAS FÍSICAS, UCM**

This seminar focuses on a series of anti-perovskites and rare-earth nitrides, including YScO_3 , LaScO_3 , PrMnO_3 , NdMnO_3 , KMgO_3 , AlNLa_3 , GaNLa_3 , and YN within a DFT/DFPT study. Their structural, electronic, mechanical, optical, and thermoelectric properties are systematically investigated. All compounds are confirmed to be both structurally and mechanically stable. Their properties exhibit a strong dependence on chemical composition and crystal structure.

The materials display a diverse range of electronic and magnetic behaviors, including semiconducting, correlated magnetic, and half-metallic states. Particularly, KMgO_3 shows full spin polarization, making it mainly promising for spintronic devices. Several systems also demonstrate favorable thermoelectric performance and optoelectronic characteristics. Recent advances in density functional theory (DFT)-based materials design validate the relevance of these compounds for applications in spintronics and energy conversion.