**MODELING STRUCTURE AND PROPERTIES OF DOPED MANGANITES**

*Permiakova A.E.*[(1)], *Antropov A.S.*[(2)], *Ostroushko A.A.*[(1)]
[(1)] Ural Federal University
620062, Ekaterinburg, Mira st., 19
[(2)] AIRI New Materials Design
123112, Moscow, Presnenskaya emb., 6

The search for new compositions and design of complex oxide materials is an attractive scientific area with enormous opportunities and potential for technological applications. In this framework, crystalline solids contribute many branches, such as energy, superconductors, electronics, catalysis, medicine, and others. Nowadays, studies are greatly assisted by computational and data-driven approaches for accelerating new materials discovery and searching for composition−structure−property relations. Particular attention is paid to the strategies that aim to predict new stable and metastable crystalline materials. To achieve this goal, different heuristics comprising the density functional theory (DFT) calculations and high-throughput screenings of modern data collections were developed. Moreover, such combinations of methods provided reliable information on the processes in solids, such as ionic transport and deintercalation and synthesis condition effects.

REE manganites contribute significantly to the current demand for high-performance functional materials. Such phenomena as colossal magnetoresistance and magnetocaloric effects have also been discovered in them. To speed up the the design of optimal compositions, comprehensive studies of the production methods, phase compositions, structure, and properties of compounds known from the literature have been conducted. However, to date, very few compositions have been comprehensively studied, and for those that have been studied, experimental data are presented in various forms, creating difficulties in processing.

Fortunately, the possible space groups and unit sell parameters corresponding to the manganite structures have been determined, and experimental preparation of compounds using various methods is possible to verify the calculated data. Existing evolutionary algorithms are, in principle, capable of varying the chemical composition, creating new compounds/phases, and choosing the most promising candidates based on the energy landscape exploration. In practice, their computational cost is low enough to enable comprehensive modeling of the complex oxides.

In this work we developed and applied the hybrid DFT/data-driven approach for searching for new stable doped lanthanum manganite. Theoretical predictions of new stable complex oxides, their structural properties, and compositions were made and the theoretical predictions were tested experimentally. This model will allow the possibility of predicting the structure and properties to be extended to a wide range of perovskite-like materials.

*The research was carried out with the financial support of the Ministry of Science and Higher Education of the Russian Federation (FEUZ-2026-0011).*