Exploring novel phases in the nickel-oxygen binary system with evolutionary algorithms and density functional theory modeling

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Transition metal oxides present a vast array of materials with innumerable technical and chemical applications. Recently, binary oxides of nickel have attracted significant attention due to their emergence as a family of new superconducting materials, as well as their relevance in various industrial processes, such as metallurgy, catalysis, and semiconductor fabrication. Known binary nickel oxides have a wide application area, and the prediction and description of new phases in Ni-O binary system might uncover new attractive and functional materials. In our work, we explore and characterize either completely unknown or poorly characterzed phases in binary transition metal oxide system Ni-O. We utilize a methodology that integrates state-of-the-art approaches such as Density Functional Theory (DFT) calculations in combination with Evolutionary Algorithms (EA) for the theoretical prediction of structures of new phases. We focus on analyzing crystal chemistry across various stoichiometries within the Ni-O binary system, examining large datasets generated by EA+DFT to uncover statistical patterns, relationships, and preferences in the data. Our findings contribute to a deeper fundamental understanding of the nickel-oxygen binary system.

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