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First-principles study of the properties of oxygen-deficient LaNiO_{3-x} structures ANDREI MALASHEVICH, SOHRAB ISMAIL-BEIGI, Center for Research on Interface Structures and Phenomena and Department of Applied Physics, Yale University — There has been a great deal of recent interest and activity regarding rare earth nickelates in bulk form, as superlattices, and as thin films. The parent nickelate in these cases is typically LaNiO_3 , which in bulk form is a paramagnetic metal. In addition, due to its relatively good lattice match to other perovskites, it also serves as an electrode in functional oxide film devices. However, it is known that the conductivity of LaNiO_3 in any form is strongly affected by the presence of oxygen vacancies. Here, we present a first-principles study of a variety of oxygen-deficient LaNiO_{3-x} structures. We describe our theoretical results for the atomic-scale geometry and energetics of the vacancies (formation and aggregation), their mobilities, and their electronic structure.

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