

Abstract Submitted
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Calculated properties of the $\text{La}_{2-2x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7$ bilayer manganites, $0.30 \leq x \leq 0.50$ ¹ ROLANDO SANIZ, ARTHUR FREEMAN, Northwestern University, MICHAEL NORMAN, Argonne National Laboratory — The low temperature properties of the $\text{La}_{2-2x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7$, $0.30 \leq x \leq 0.50$ bilayer manganites have been studied in the past using a host of experimental techniques in order to understand the outstanding phenomena they exhibit. To complement these investigations, we present a systematic study of their calculated ground state properties as a function of doping level, using the highly precise full-potential linearized augmented plane wave (FLAPW) method,² and focusing on magnetic order and optical and transport properties. Our results, which are in very good agreement with experiment in several respects, underline the correlation between the structural and orbital degrees of freedom and also shed light on many of the unexpected observations at low temperature in angle-resolved photoemission spectroscopy, optical conductivity, and resistivity measurements.

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²Wimmer, Krakauer, Weinert, Freeman, Phys.Rev.B, **24**, 864 (1981).

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