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Strain control of spin and orbital transitions in La_2NiO_4 CHOONG H. KIM, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — We have studied the electronic and magnetic structure of the layered nickelates, La_2NiO_4 within density functional theory. We show that biaxial strain induces a high spin to low spin transition, which coincides with a significant change in the $x^2 - y$ and $3z^2 - r^2$ orbital occupancy. We discuss the role of the on-site Coulomb interaction, the crystal field, and prospects for the strain control of the spin and orbital state.

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