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**Lattice relaxation, electronic screening, and spin and orbital phase diagram of $LaTiO_3/SrTiO_3$ superlattices** SATOSHI OKAMOTO, ANDREW MILLIS, Department of Physics, Columbia University, NICOLA SPALDIN, Materials Department, University of California, Santa Barbara — The effect of lattice relaxation on the electronic charge density, band structure, and phase diagram in oxide heterostructure, $LaTiO_3/SrTiO_3$ superlattices, the structure grown and measured by Ohtomo *et al.*[1], is investigated using density functional theory LDA and LDA+$U$ (VASP implementation). We observe substantial ferroelectric-like distortion of $TiO_6$ octahedra at the nearest-to-La region which screens the electrostatic force originating from $La^{3+}$ ion reducing the charge density in the La-rich region. We determine the changes in the low energy electronic Hamiltonian caused by the lattice relaxation and investigate the consequences for the ground state phase diagram using the Hartree-Fock approximation. Finally, we present a detailed comparison with previous calculations which neglected the lattice effect. [2] Support from DOE ER 46169. [1]Ohtomo et al., Nature **419**, 378 (2002). [2]Okamoto and Millis, Nature (London) **428**, 630 (2004), and Phys. Rev. B **70**, 195120 (2004).

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