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The persistence of ferroelectric distortions in electron-doped BaTiO3: microscopic origins and critical behavior YONG WANG, JOHN BURTON, SITARAM JASWAL, EVGENY TSYMBAL, University of Nebraska - Lincoln — To explore possible novel applications of the prototypical ferroelectric oxides we perform theoretical studies of electron-doping in BaTiO3. The presence of conduction electrons in a ferroelectric opens the possibility of bi-stable behavior directly in a conducting material which may lead to new functionalities. It is known, however, that conduction electrons screen the long range Coulomb interactions responsible for polar instabilities. Interestingly though, our first-principle density functional calculations reveal that ferroelectric distortions can persist in electron-doped BaTiO3 up to 0.01 e/unit cell, consistent with experimental results [1], suggesting that ferroelectricity and conductivity can coexist. To elucidate the competition between the long range Coulomb interactions and the short range bonding effects we have developed an adequate electrostatic model. Using this model, we reproduce the polarization vs. doping behavior obtained from first-principles and derive an analytical expression for the critical doping above which ferroelectric distortions disappear. [1] T. Kolodiazhnyi et al, Phys. Rev. Lett. 104, 147602 (2010).

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