

Abstract Submitted
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Evaluating Born and local effective charges in nanoscale MnO¹

Q.-C. SUN, X.S. XU, University of Tennessee, S.N. BAKER, A.D. CHRISTIANSON, Oak Ridge National Laboratory, J.L. MUSFELDT, University of Tennessee — Phonons are exquisitely sensitive to finite length scale effects in complex materials because they are intimately connected to charge, polarizability, and structure, and a quantitative analysis of their behavior can reveal microscopic aspects of chemical bonding. To investigate these effects in a model correlated oxide, we measured the infrared vibrational properties of 8 nm particles of MnO, compared the results with the analogous bulk material, and quantified the phonon confinement with a calculation of Born effective charge. Our analysis reveals that the Born effective charge decreases by $\sim 20\%$ compared to the bulk material. This finding is important for understanding finite length scale effects in this simple binary oxide and the more complicated functional oxides that emanate from this parent compound.

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