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**Nanoscale structural and electronic characterization of $\alpha$-$RuCl_3$ layered compound**[1] MAXIM ZIATDINOV, ARTEM MAKSOV, ARNAB BANERJEE, WU ZHOU, TOM BERLIJN, JIAQIANG YAN, STEPHEN NAGLER, Oak Ridge National Laboratory, DAVID MANDRUS, University of Tennessee, ARTHUR BADDORF, SERGEI KALININ, Oak Ridge National Laboratory
— The exceptional interplay of spin-orbit effects, Coulomb interaction, and electron–lattice coupling is expected to produce an elaborate phase space of $\alpha$-$RuCl_3$ layered compound, which to date remains largely unexplored. Here we employ a combination of scanning transmission electron microscopy (STEM) and scanning tunneling microscopy (STM) for detailed evaluation of the system's microscopic structural and electronic orders with a sub-nanometer precision. The STM and STEM measurements are further supported by neutron scattering, X-Ray diffraction, density functional theory (DFT), and multivariate statistical analysis. Our results show a trigonal distortion of Cl octahedral ligand cage along the $C_3$ symmetry axes in each $RuCl_3$ layer. The lattice distortion is limited mainly to the Cl subsystem leaving the Ru honeycomb lattice nearly intact. The STM topographic and spectroscopic characterization reveals an intra unit cell electronic symmetry breaking in a spin-orbit coupled Mott insulating phase on the Cl-terminated surface of $\alpha$-$RuCl_3$. The associated long-range charge order (CO) pattern is linked to a surface component of Cl cage distortion. We finally discuss a fine structure of CO and its potential relation to variations of average unit cell geometries found in multivariate analysis of STEM data.

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