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Abstract for an Invited Paper for the MAR16 Meeting of the American Physical Society

Single atom electrochemical and atomic analytics¹ RAMA VASUDEVAN², Oak Ridge National Laboratory

In the past decade, advances in electron and scanning-probe based microscopies have led to a wealth of imaging and spectroscopic data with atomic resolution, yielding substantial insight into local physics and chemistry in a diverse range of systems such as oxide catalysts, multiferroics, manganites, and 2D materials. However, typical analysis of atomically resolved images is limited, despite the fact that image intensities and distortions of the atoms from their idealized positions contain unique information on the physical and chemical properties inherent to the system. Here, we present approaches to data mine atomically resolved images in oxides, specifically in the hole-doped manganite La5/8Ca3/8MnO3, on epitaxial films studied by in-situ scanning tunnelling microscopy (STM). Through application of bias to the STM tip, atomic-scale electrochemistry is demonstrated on the manganite surface. STM images are then further analyzed through a suite of algorithms including 2D autocorrelations, sliding window Fourier transforms, and others, and can be combined with basic thermodynamic modelling to reveal relevant physical and chemical descriptors including segregation energies, existence and strength of atomic-scale diffusion barriers, surface energies and sub-surface chemical species identification. These approaches promise to provide tremendous insights from atomically resolved functional imaging, can provide relevant thermodynamic parameters, and auger well for use with first-principles calculations to yield quantitative atomic-level chemical identification and structure-property relations.

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