Quantitative Imaging of Atomic-Scale Chemistry Changes at Interfaces

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NEW

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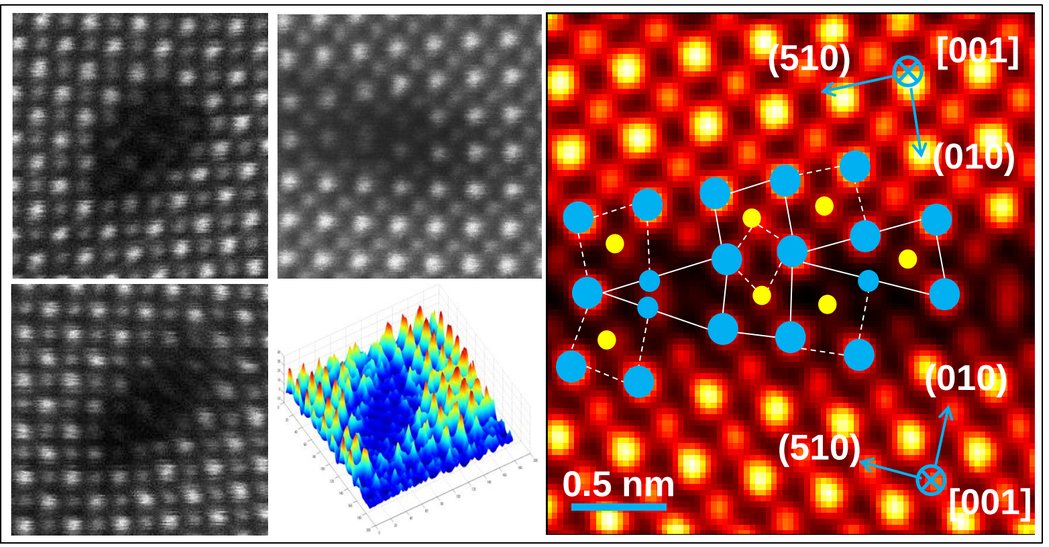
Purpose

Develop a robust method to ***quantify*** atomic-scale changes in structure, composition, and bonding at interfaces.

This research will use the advanced capabilities for chemical imaging under varied environmental conditions afforded by the new generation of aberration-corrected microscopes and *in situ* stages.

Structure-Chemistry-Properties

Given the wealth of information generated by aberration-corrected microscopes, analysis methods can now move beyond single images and test structural variance over large areas of interface. This variance identifies key locations in the structure and a probability map of atom locations. These maps are comparable to DFT calculations, allowing an atomic-scale understanding of the interplay between structure-chemistry and properties to be developed.



Expected Outcomes

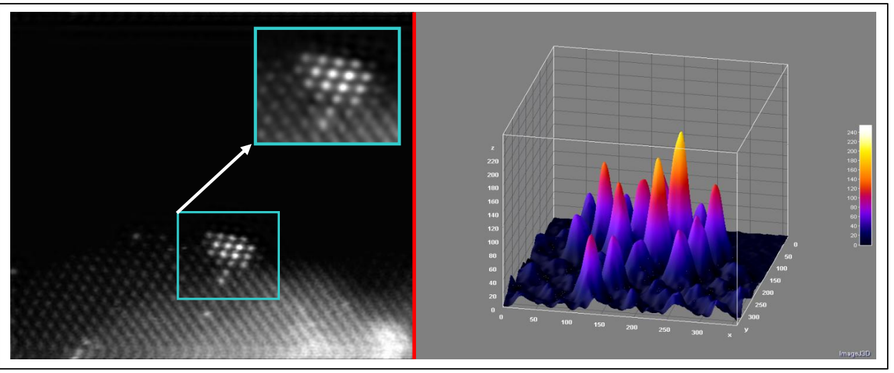
Develop robust statistical methods for reproducible and quantified image analysis/interpretation

Apply methods to understand the interplay of structure-composition and properties at interfaces in functional oxides

Apply these statistical methods to investigate heterogeneous catalysts

Nanoscale Catalysts

Aberration-corrected STEM gives unprecedented information on the atomic content and distribution of nanoscale clusters used for catalysis. The difficulty is keeping the electron dose down to a level where the clusters remain stationary and intact. When low-dose techniques are employed using *in situ* gas stages, complete 3D distributions of atoms within nanoclusters can be obtained as a function of environmental conditions.



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