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Crystal Interface Lab. Seminar Series

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New solutions to the energy crisis through aberration-corrected STEM

by

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Aberration-corrected STEM has improved lateral resolution by more than a factor of two, giving single atom semsitivity for both imaging and EELS. In addition, it is possible to obtain simultaneous, aberration-corrected phase contrast and Z-contrast images, so the complementary characteristics of each can be combined. Aberration-correction allows much larger probe-forming apertures to be used, which results in a much decreased depth of field. Structural information can now be extracted in three dimensions by optical sectioning, with sub-Ångström lateral resolution and a depth resolution of a few nanometers. These same advantages apply to EELS, limited somewhat by delocalization of the inelastic interaction, but primarily by the lower signal.

These benefits will be illustrated by several case studies in different areas of materials, with emphasis on energy applications. In catalysis, single atom sensitivity in 3D enables a link to catalytic activity through density functional calculations. The high activity of nanophase gold clusters on titania can be quantitatively explained. In semiconductors, individual Hf atoms have been located within a $Si/SiO_2/HfO_2$ gate dielectric structure to a precision of 0.1 x 0.1 x 1 nm, and the perturbed electronic structure linked by density functional theory to macroscopic device properties. Column-by-column compositional mapping of InAsP quantum wires coupled to elasticity calculations explains their growth morphology and optical properties. In Si nanowires individual gold atoms have been imaged *inside* the wire in several substitutional and interstitial configurations, with number densities that are in order of calculated formation energies.

In future, new probes of materials functionality could be added to the aberration-corrected STEM, allowing direct mapping of properties while maintaing the unprecedented capability for atomic and electronic structure determination. Addition of a cathodoluminescence detector would allow light emission to be mapped in materials for solid state lighting, providing direct correlation to local defects such as dislocations or interface steps. In solar cells, electron beam induced current could provide maps of charge collection efficiency, locating and characterizing poorly functioning interfaces. Addition of a scanning tunnelling microscope inside the STEM would allow bias to be applied to interfaces, band bending effects to be introduced, and the effect on local functionality to be explored. In catalysis, thin window, in-situ cells could maintain atomic resolution in high pressure or corrosive environments. All of these new probes would greatly extend our ability to probe energy conversion processes in materials, and through theory, understand the limitations and overcome them at the fundamental quantum level.

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