Engineering Smart Materials via Atomic-resolution Microscopy and Spectroscopy

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Abstract- The development of smart catalysts, piezoelectrics, thermoelectrics, light emitting diodes and 2D materials and devices is increasingly important in addressing environmental and energy concerns. The powerful combination of aberration-corrected microscopy and theoretical calculations allows a direct correlation of atomic-scale structure and bonding to materials' properties, representing a new and efficient approach to materials' development. A number of illustrative examples will be presented.

In catalysis, it has become almost routine to image single atoms and probe their bonding by spectroscopy, greatly aiding development of single atom catalysts (SACs). Their unique coordination can impart exceptional activity and selectivity, and much effort is ongoing to replace platinum group metals by cheaper, earth abundant metals such as cobalt or nickel.[1] Examples include a Co SAC with good activity for both the oxygen evolution and oxygen reduction reactions, and its application as the air cathode in a solid-state Zn−air battery.[2]

In nitride-based light-emitting materials, development of an efficient green/red emitting system would further enhance efficiency, but is hampered by the large misfit of high In content $Ga_xIn_{1-x}N$ on GaN. Recently, by understanding the nucleation of defects, a 9-fold improvement in emission efficiency has been achieved.

Improved lead-free piezoelectric materials are also urgently required. By employing atomic-resolution polarization mapping we can uncover the general structural requirements, a coexistence of ferroelectric phases inside nanodomains, and have significantly enhanced the properties of $(K,Na)NbO_3$ and $BaTiO_3$ based lead-free piezoceramics.[3-5] Nanostructuring is also widely used to enhance thermoelectric properties. Direct observation of intrinsic Pb vacancies and extrinsic Cu interstitials in PbTe reveals the mechanism underlying the optimization of phonon and carrier transport.[6] Recently, doping S into SnSe has markedly improved performance, representing an important step toward low-cost, earth-abundant, environmentally friendly thermoelectrics.[7]

In 2D materials, configurations of point defects and their local environments can be directly identified and correlated with properties.[8] It is also possible to selectively sputter light atoms leaving heavier metals atoms intact. In this way we fabricated suspended monolayer Mo membranes from monolayer $MoSe_2$ films, and directly imaged their formation mechanism.[9]

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Keywords- Catalysts, piezoelectrics, thermoelectrics, light emitting diodes, 2D materials.