and BaTiO$_3$ is a metal whereas BaTi$_{1-x}$Nb$_x$O$_3$ is insulating, despite being very similar structurally and electronically. However neutron PDF studies reveal the 8a compound to be locally distorted, like rhombohedral BaTiO$_3$.

### Size effects in BaTiO$_3$

Three different sizes of BaTiO$_3$ nanoparticles; 26 nm, 45 nm, and 70 nm, have been studied by synchrotron diffraction. All samples are reliably tetragonal, but the tetragonal distortion becomes much smaller as particle size decreases. The off-centering of Ti in the Pmnn cell however increases with decreasing particle size.

### Tuning magnetism in insulating spinels

With two Jahn-Teller active ions, and a plethora of interesting magnetic interactions, the spinel structure provides a laboratory for exploring complex magnetic ground states. The data shown here suggests how magnetic ground states can be tuned in the system $\text{Zn}_2\text{Mn}_2\text{O}_4$.

### The structure of Mg-doped ZnO

This is an important problem in terms of how the static polarization of ZnO changes with Mg-substitution. PDF studies have helped unravel subtle structural details with unprecedented accuracy, and to make comparison with DFT results on the hypothetical wurzbiltte MgO.

### Density functional theory visualization of lone pairs

We make extensive use of density functional calculations in order to better understand structural phenomena in solids, in particularly those deriving from the stereochromic activity of lone pairs of electrons in the lower-valet cations of the heavier main group elements (P$^5+$, Bi$^6+$ etc.).

### Unraveling the locus of atom positions in Cu$_2$O

With two Jahn-Teller active ions, and site disorder, the spinel Cu$_2$O provides a great challenge to modern methods of structural analysis. Reverse Monte Carlo analysis of time-of-flight neutron scattering reveals the surprising result that Cu$^{+}$ partially disproporionsates to Cu$^0$ and Cu$^2+$ in order to avoid JT distortions.

### Model compounds for catalysis by PGM ions

Heterogeneous catalysis by platinum group metal (PGM) ions is exceedingly important in numerous industrial processes, as well as in 3-way catalysis in automobiles. The scarcity of PGMs has motivated us to examine links between crystal chemistry and catalysis, including in unusual Au$^+$ compounds, such as La$_2$(Au$_2$O$_6$)$_2$ whose structure and XPS spectrum are shown here.

### New Ce$^{3+}$ phosphors for solid state lighting

Light-emitting diodes based on (In,Ga)N are revolutionizing lighting, with the potential of saving many billions of dollars in energy every year. A key component in (In,Ga)N-based white lighting is an organic phosphor for conversion of blue and UV emission from (In,Ga)N to a broad, high rendition white.