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## Guest Lecture

**Title:** "Synthesizing Designer Oxides as Thin Films – the Transition Metal Calls the Shots!"

**Speaker:** Dr. Scott A. Chambers

**Address:** Physical Sciences Division, Pacific Northwest National Laboratory  
Richland, WA USA

**Date:** Friday, 6<sup>th</sup> of June 2014

**Time:** 14:30

**Place:** Seminar Room CBEG02 (387, Photonics); Gußhausstraße 27

### Abstract:

SrCrO<sub>3</sub> is the least explored, and most controversial of the first-row transition metal complex oxides. There are conflicting reports in the literature concerning its electronic and magnetic properties. Our opinion is that the controversy stems from the use of compositionally and structurally ill-defined polycrystalline materials.

In order to synthesize structurally and compositionally well-defined SrCrO<sub>3</sub> and explore its properties, we have attempted to deposit SrCrO<sub>3</sub> as thin crystalline films on lattice matched perovskite substrates using molecular beam epitaxy (MBE), which is generally considered to be the most highly controlled method for thin-film synthesis, and to result in materials of the higher purity and lowest defect density. Yet, despite our efforts, what actually nucleates under optimal conditions is semiconducting, rhombohedral SrCrO<sub>2.8</sub> rather than cubic, perovskite, metallic SrCrO<sub>3</sub>. The reason SrCrO<sub>2.8</sub> nucleates is that Cr<sup>4+</sup> is not stable in an octahedral coordination environment, and



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kinetic limitations associated with the MBE growth process preclude the formation of fully oxidized  $\text{SrCrO}_3$ . However, as-grown  $\text{SrCrO}_{2.8}$  phase can be transformed, reversibly and at low temperature, to metallic perovskite  $\text{SrCrO}_3$  by gentle annealing in air. Oxygen vacancies in  $\text{SrCrO}_{2.8}$  aggregate and give rise to ordered arrays of {111}-oriented  $\text{SrO}_2$  planes interleaved between layers of tetrahedrally-coordinated  $\text{Cr}^{4+}$  and separated by  $\sim 1$  nm. These oxygen-deficient  $\text{SrO}_2$  planes constitute fast diffusion paths for  $\text{O}^{2-}$ , allowing easy oxidation to  $\text{SrCrO}_3$ .

First-principle calculations provide insight into the origin of the stability of these nanostructures and, consistent with the experimental data, predict that the barrier for  $\text{O}^{2-}$  diffusion along these quasi-2D nanostructures is  $\sim 4$  times lower than that in the cubic  $\text{SrCrO}_3$ . This property is of considerable importance in solid oxide fuel cells where fast  $\text{O}^{2-}$  diffusion reduces the required operating temperature.