Materials Research Science and Engineering Centers, DMR-1720415

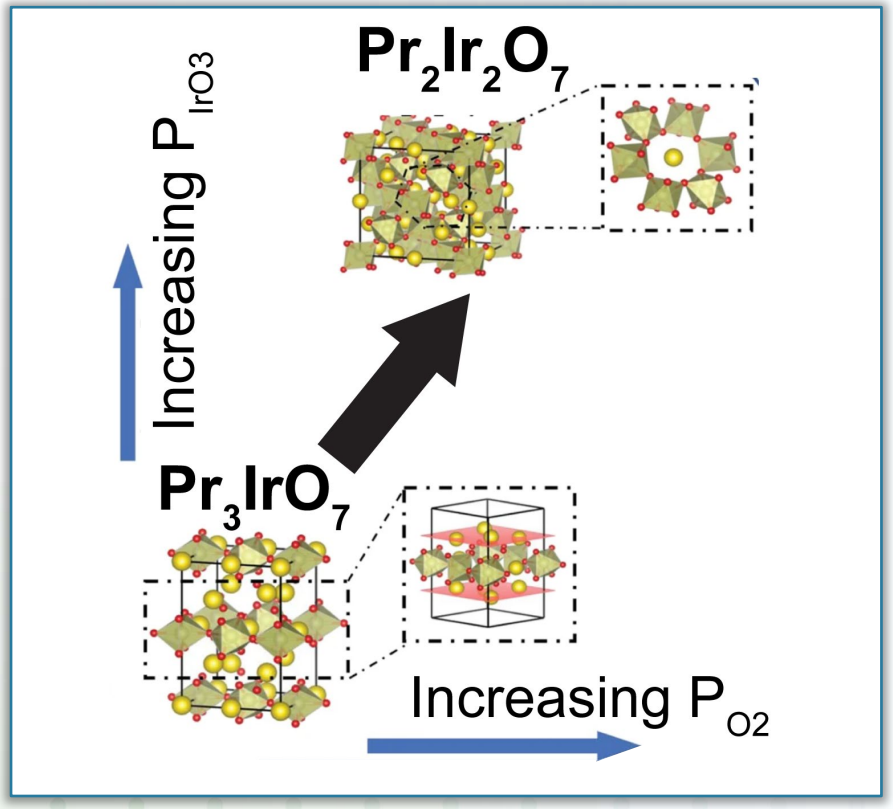
IRG 2, 2021

Computationally designed synthesis of complex oxide materials

Paul G. Evans, Chang-Beom Eom
University of Wisconsin-Madison

The useful properties of chemical compounds are determined by the elements from which they are made and the arrangement of the atoms. However, there are often several ways atoms of the same elements can be arranged to form a solid. Wisconsin MRSEC researchers are particularly interested in a series of compounds formed from rare-earth elements and iridium. One phase, $Pr_2Ir_2O_7$, is of particular interest because it exhibits novel magnetic phenomena and can open new opportunities in the field of quantum materials.

Using computer simulations, the MRSEC researchers discovered conditions that favor the formation of the desired $Pr_2Ir_2O_7$ phase and make the competing phases with the same elements, such as Pr_3IrO_7, less favorable. The specific favorable conditions include changing the pressures of IrO_3 and O_2 gas during the synthesis process, P_{IrO3} and P_{O2}. The results allow researchers to form $Pr_2Ir_2O_7$ using precisely controlled crystal growth conditions and will broaden the use of this class of compounds.



Synthesis of $Pr_2Ir_2O_7$ is complicated by the presence of competing Pr_3IrO_7 phases. $Pr_2Ir_2O_7$ is favored through the selection of thermodynamic parameters including the O_2 and IrO_3 partial pressures.

NSF DMR DIVISION OF MATERIALS RESEARCH
DIRECTORATE FOR MATHEMATICAL AND PHYSICAL SCIENCES

Lu Guo, Shun-Li Shang, Neil Campbell, Paul G. Evans, Mark Rzchowski, Zi-Kui Liu, and Chang-Beom Eom, "Searching for a route to synthesize in situ epitaxial $Pr_2Ir_2O_7$ thin films with thermodynamic methods," NPJ Computational Materials **7**, 144 (2021).