The Role of Local Structure in the Optical Properties of Hexagonal $YMn_{1-x}Ga_xO_3$ and Isostructural Compounds

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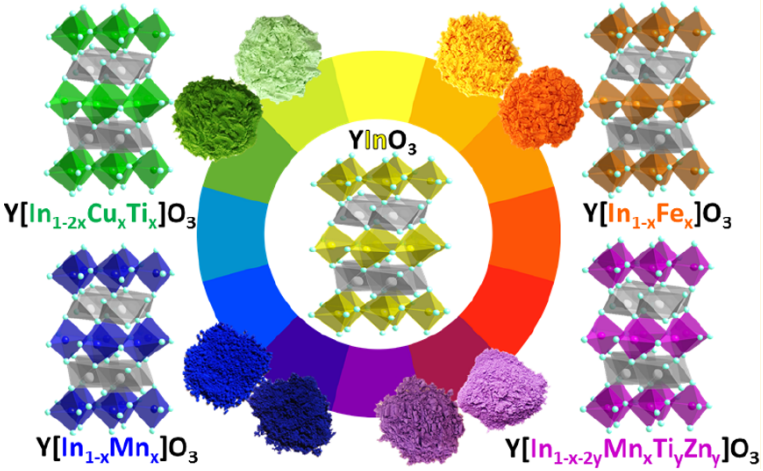
Chromophores based on $YInO_3$



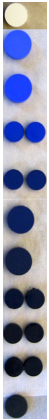
Base compound is white, dopant gives intense colors

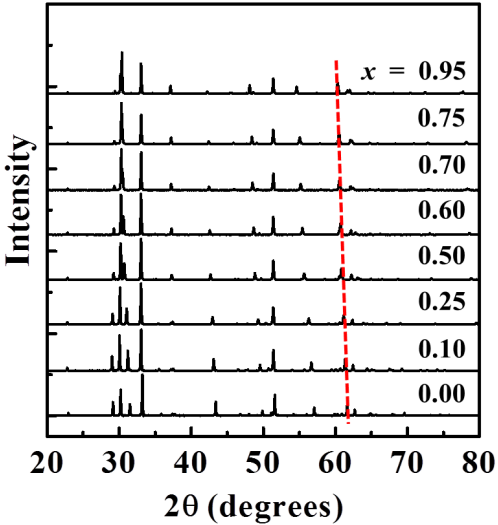
The Mn variant has commercial promise

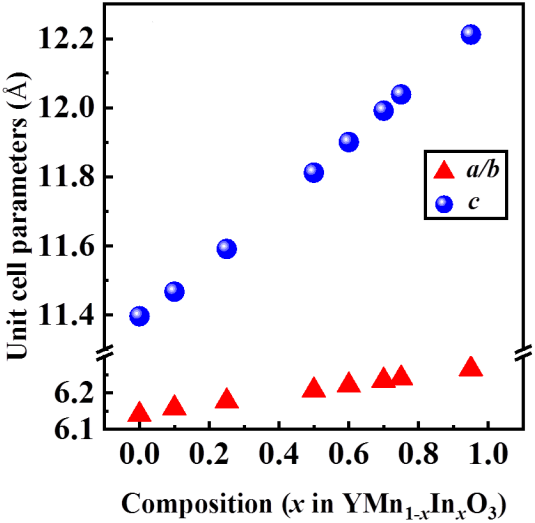
Hexagonal structure with YO_6 octahedra and InO_5 trigonal bipyramids

J. Li, S. Lorger, J.K. Stalick, A.W. Sleight, and M.A. Subramanian, *Inorg. Chem.* **55**, 9798–9804 (2016).

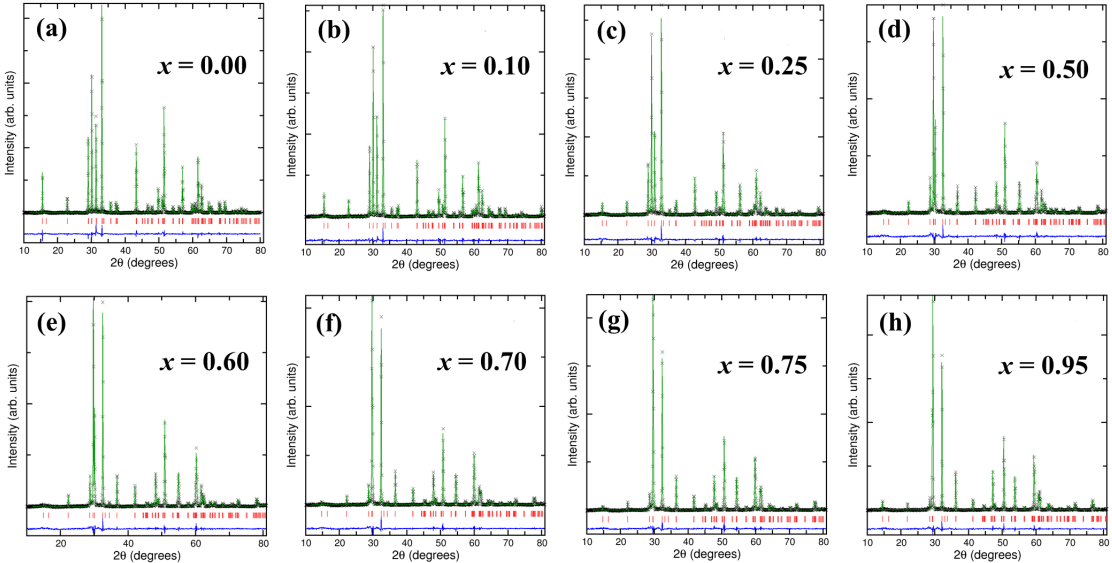
$YMn_{1-x}In_xO_3$ solid solution



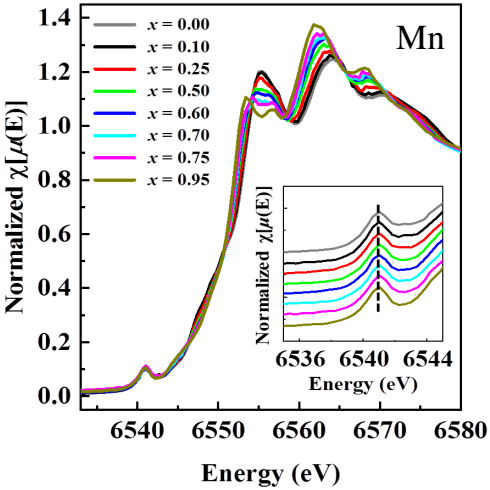


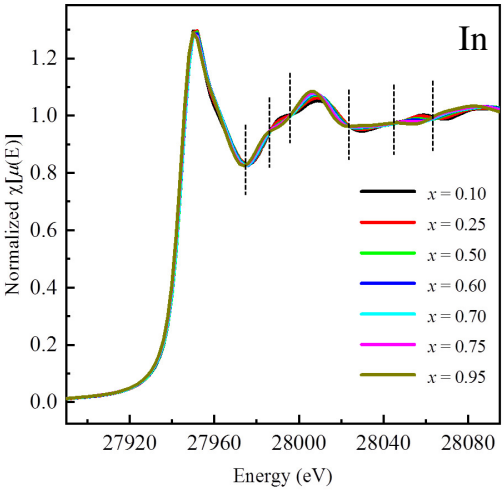


$YMn_{1-x}In_xO_3$ refinements

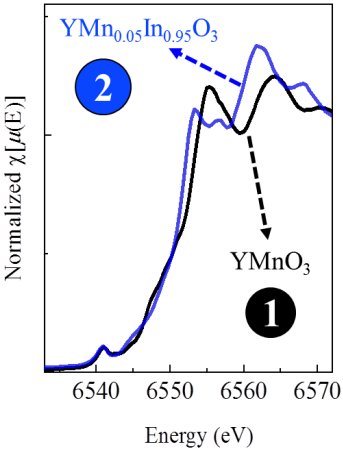


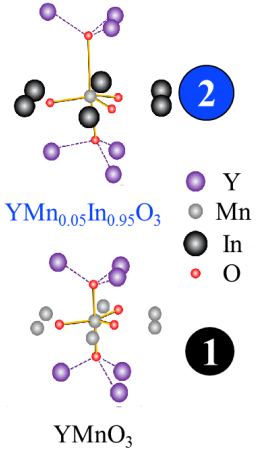
$YMn_{1-x}In_xO_3$ x-ray absorption spectroscopy

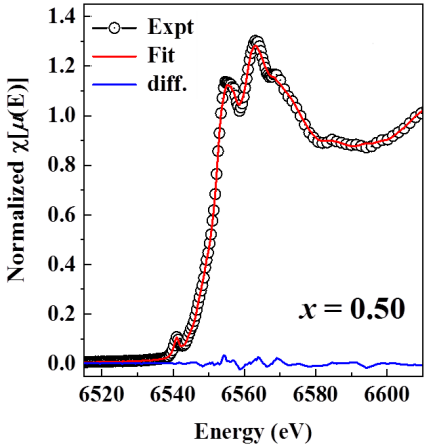




Bimodal Mn local environment fits XANES

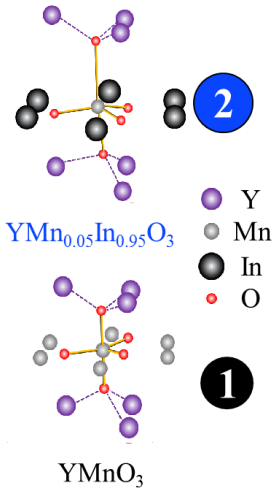


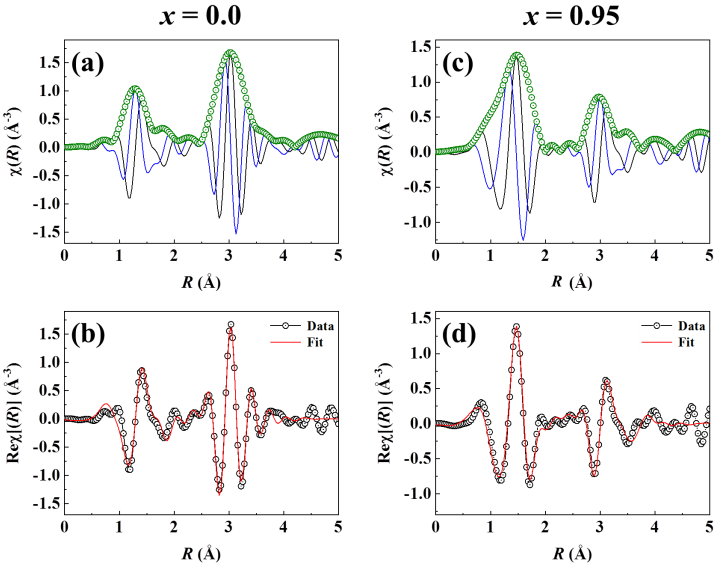




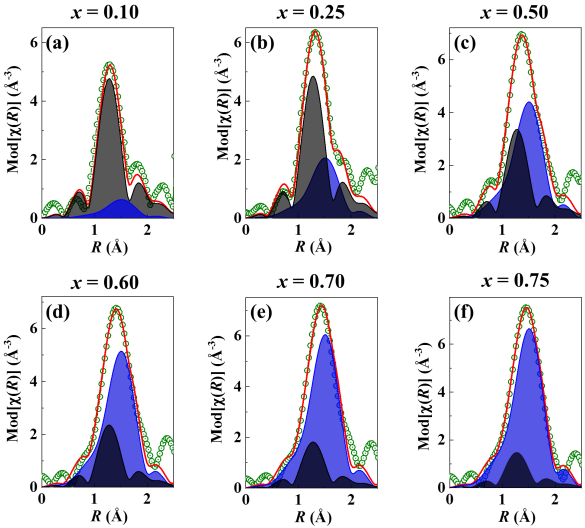
S. Mukherjee, H. Ganegoda, A. Kumar, S. Pal, C.U. Segre, and D.D. Sarma, *Inorg. Chem.* **57**, 9012–9019 (2018).

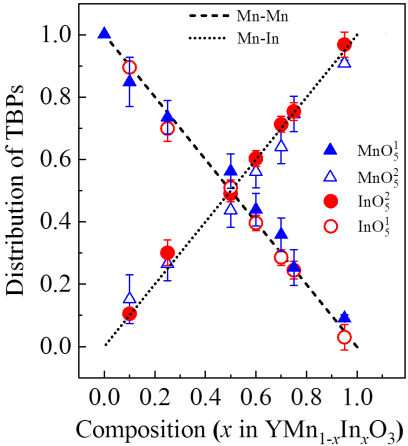
Detailed modeling on endpoint composition



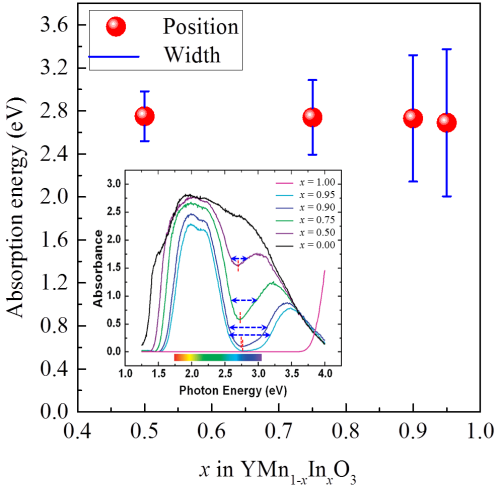


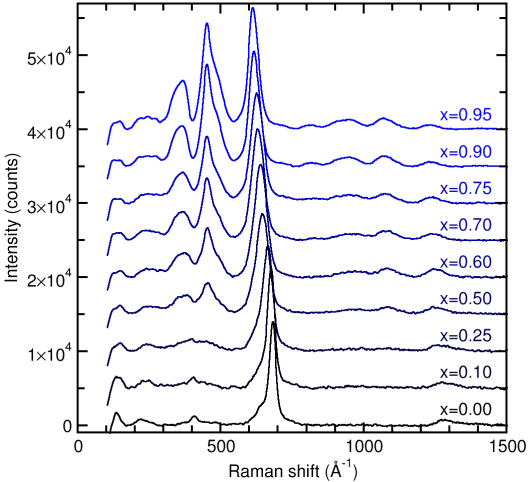
Endpoint EXAFS fits describe all samples





$YMn_{1-x}In_xO_3$ optical properties





Purple $YMn_{1-x}Ga_xO_3$ solid solution

$YGaO_3$ has same hexagonal structure

Doping with Mn gives brilliant purple colors

Is Mn in a bimodal local environment?

$YMn_{1-x}Ga_xO_3$ is more challenging, requiring careful control of temperature and time to avoid garnet impurity phase

x=0.70 x=0.80 x=0.90 x=0.95 x=0.98

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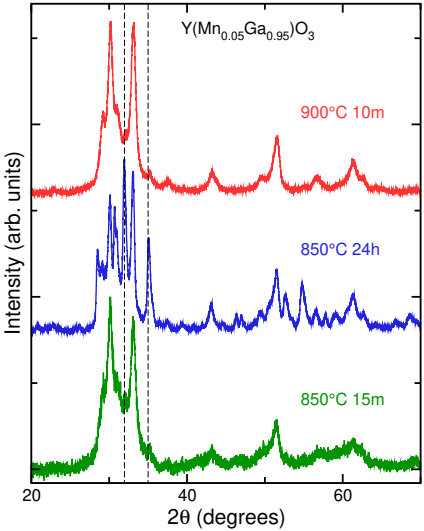
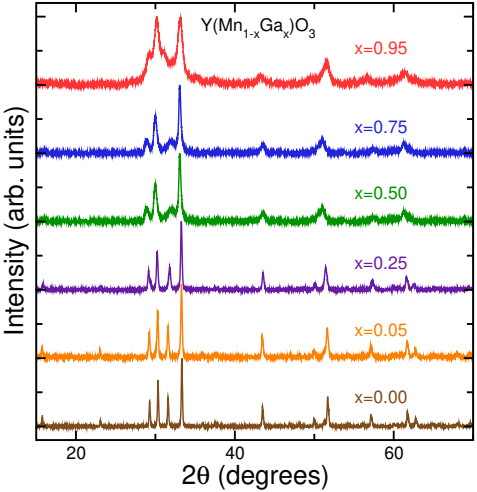
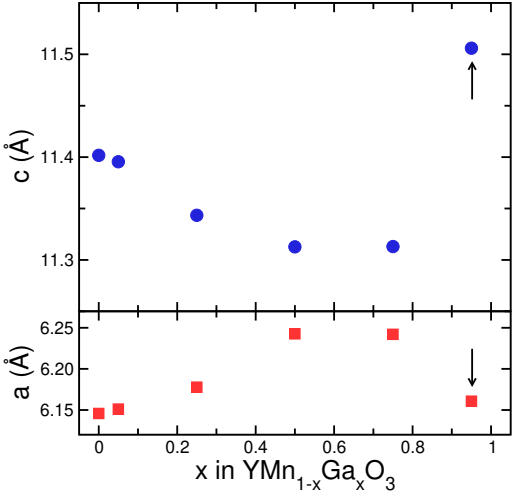
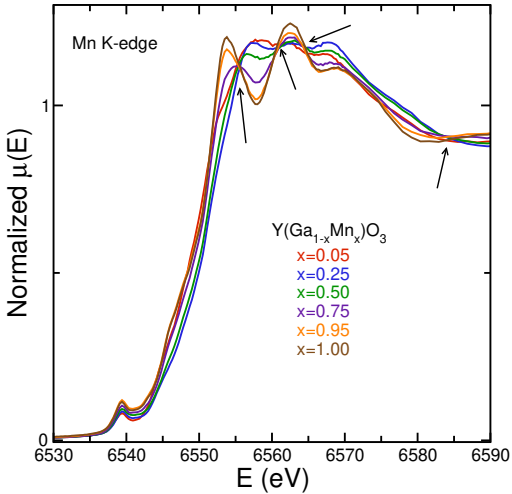


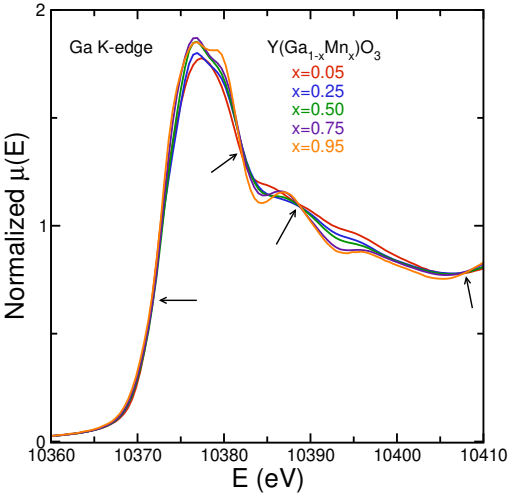
$YMn_{1-x}Ga_xO_3$ diffraction data



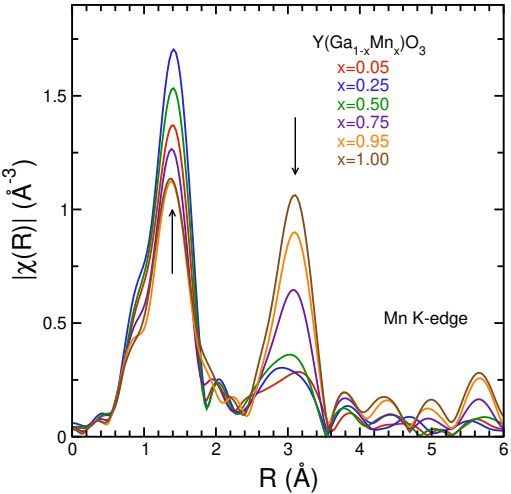


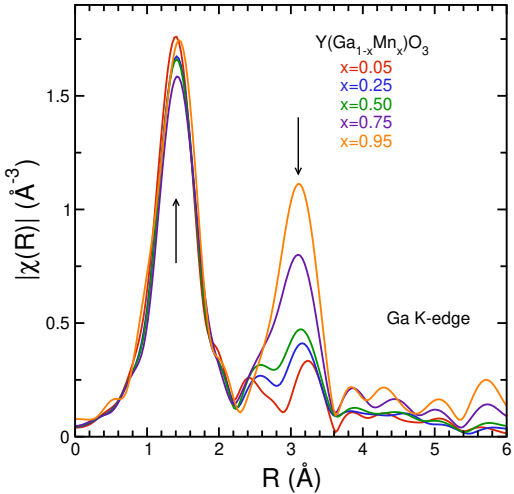
$YMn_{1-x}Ga_xO_3$ XANES





$YMn_{1-x}Ga_xO_3$ EXAFS





Where do we go from here?

$YMn_{1-x}Ga_xO_3$ needs additional work to obtain good crystalline samples across the composition range

Bimodal environments seem to be a general property of the two systems studied so far

Will this bimodal environment be present in all systems based on this hexagonal structure? In other chromophore systems?

May need to revisit local structural effects in other such oxide systems

Collaborators & Acknowledgements

Huanbo Sun – Illinois Tech

Soham Mukherjee – Uppsala University

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