

## Colloquium

### **Rational design of functional materials: A chemist's approach**

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New functional materials can be designed by interplay of synthesis and crystallographic structure. Unconventional synthetic routes play an important role in this direction as many of these new materials are metastable and hence it is not possible to prepare them by conventional synthesis methods. Of late, the focus of research has been shifted to multi-functional materials i.e., the materials which can possess two or more than two synergistic or antagonistic functionalities. The synthesis of such materials has been a challenge and also an opportunity to chemists. We have prepared a number of new functional materials guided by crystallographic approach coupled with novel synthesis protocols. Some typical materials which will be discussed in this talk are  $\text{La}_{1-x}\text{Ce}_x\text{CrO}_3$ ,  $\text{Pr}_{1-x}\text{Ce}_x\text{ScO}_3$  (materials with tunable band gap and magnetic properties),  $\text{CeScO}_3$  (with unusual reversible conversion to fluorite lattice),  $\text{Gd}_{1-x}\text{Y}_x\text{InO}_3$ ,  $\text{GdSc}_{1-x}\text{In}_x\text{O}_3$ ,  $\text{YIn}_{1-x}\text{Fe}_x\text{O}_3$  (tunable dielectrics) and several lead free relaxor materials. Perovskite and fluorite-type materials with trivalent  $\text{Ce}^{3+}$  were successfully prepared from suitable precursor powders by a controlled heating under low  $\text{PO}_2$ . Several interesting pyrochlore based oxygen storage materials, viz.  $\text{Ce}_2\text{Zr}_2\text{O}_{7+x}$  ( $x = 0.0$  to  $1.0$ ),  $\text{Gd}_{2-x}\text{Ce}_x\text{Zr}_2\text{O}_7$  and  $\text{Gd}_{2-x}\text{Ce}_x\text{Zr}_{2-x}\text{Al}_x\text{O}_7$  ( $x = 0.0$  to  $2.0$ ) have been prepared, which have shown interesting redox catalysis. The simple concepts like  $r_A/r_B$  ratio of  $\text{A}_2\text{B}_2\text{O}_7$  pyrochlores could be used to tailor the properties like ionic conductivity, dielectric and photocatalytic behavior. The major focus of this talk will be on the role of synthesis, novel properties exhibited by these functional materials, and their crystallographic correlation.

**Monday, Mar 18<sup>th</sup> 2019**

**4:00 PM (Tea/Coffee at 3:30 PM)**

**Auditorium, TIFR-H**