

Mixed anion compounds with functional properties

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Mixed anion compounds such as oxychlorides, oxychalcogenides, oxyhydrides and oxynitrides are an emerging class of materials with intriguing properties, including solar-activated photocatalyst BaTaO_2N , high-temperature superconducting iron pnictides, EuNbO_2N with colossal magnetoresistance, spin liquid system $(\text{CuCl})\text{LaNb}_2\text{O}_7$ and transparent p-type semiconducting system LaCuOS , to name only a few.

My talk will mostly focus on the synthesis, structure and properties of several transition-metal oxyhydrides. $\text{ATi}(\text{O},\text{H})_3$ (A = alkali metal) can be obtained in a topochemical fashion using CaH_2 reduction of the corresponding oxide hosts [1]. $\text{ATi}(\text{O},\text{H})_3$ is metallic with high carrier concentrations, though it fails to be superconducting at least down to 0.5 K [2]. Besides, hydride (H^-) ions are quite mobile at moderate temperatures, implying potentials of the oxyhydrides as ionic conductors and catalysts. Multistep reactions via oxyhydride will also be shown.

Mixed anion perovskite-based structures such as SrCrO_2H and MnTaO_2N can be prepared by high temperature and high pressure reaction [3, 4]. For SrCrO_2H , despite the non-bonding nature in Cr 3d and H 1s orbitals, the magnetic order temperature is as high as 380 K, which is significantly higher than those in isoelectric (Cr^{3+}, d^3) with LnCrO_3 (Ln = rare earth). This can be reasonably explained by octahedral tilting scheme.

We have prepared new titanium oxypnictides $\text{BaTi}_2\text{Sb}_2\text{O}$ and $\text{BaTi}_2\text{Bi}_2\text{O}$. A novel electronic phase diagram has been found in the solid solution $\text{BaTi}_2(\text{Sb},\text{Bi})_2\text{O}$, where two superconducting phases are separated by a metallic phase [5]. Similar phase diagram is also seen in high- T_c superconducting iron arsenides.

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[4] C. Tassel et al., *Angew. Chem. Int. Ed.* **54**, 516 (2015).

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Fields of Research

Solid State Chemistry, Solid State Physics

Publications

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