Mihai I Sturza et al., J Material Sci Eng 2018, Volume 7
DOI: 10.4172/2169-0022-C5-105

Novel low dimensional mixed valent transition metal chalcogenides discovered by exploratory synthesis

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The class of transition-metal chalcogenides that exhibits mixed valency has been of continuing interest for several decades. The emergence of superconductivity with a superconducting transition temperature (Tc<30 K) in mixed-valence $AxFe_2$–ySe_2 (A=K, Rb, Cs, and Tl) phases has further increased interest in the chemistry and physics of complex ternary transition-metal chalcogenides. Copper chalcogenide materials are of considerable scientific interest because of their rich structural and compositional diversity, mixed valency, propensity for phase transitions, charge-density waves, potential for ionic mobility, as well as applications such as high performance photovoltaic cells. New results from the chemistry of the A/Cu/Q (A=Na, K, Ba; Q=S, Se) system will be reported. The synthesis, crystal structure, and properties of new layered copper chalcogenide compounds, which are mixed-valent will be presented. Single crystals were grown by the reaction of Cu metal in a molten alkali/ alkaline-earth metal/polysulfide/polyselenide/flux. Single crystal x-ray diffraction measurements performed on several crystals showed a high quality of the crystals, proven by the good internal consistency of the data collected using the full-sphere mode and an extremely low R factor. Electronic band structure calculations and physical property measurements reveal p-type metallic behavior, with moderately high electrical conductivity and hole carrier mobilities.

Recent Publications

1. A J E Rettie, M Sturza, C D Malliakas, A S Botana, M R Norman, D Y Chung and M G Kanatzidis (2017) Copper vacancies and heavy holes in the two-dimensional semiconductor KCu_3-xSe_2. Chem. Mater. 29(14):6114–6121.
2. M Sturza, D E Bugaris, C D Malliakas, F Han, D Y Chung and M G Kanatzidis (2016) Mixed valent $NaCu_4Se_3$: A two-dimensional. Inorg. Chem. 55(10):4884-4890.
3. H J Grafe, S Nishimoto, M Iakovleva, E Vavilova, A Alfonsov, M I Sturza, S Wurmehl, H Nojiri, H Rosner, J Richter, U K Roßler, S L Drechsler, V Kataev and B Buchner (2017) Evidence for a magnetic field-induced hidden spin nematic phase in the frustrated and anisotropic spin-chain cuprate $LiCuSbO_4$. Scientific Reports 7:6720.
4. M Sturza, J M Allred, C D Malliakas, D E Bugaris, F Han, D Y Chung and M G Kanatzidis (2015) Tuning the magnetic properties of new layered iron chalcogenides $(BaF)_2Fe_2$–xQ_3 (Q=S, Se) by changing the defect concentration on the iron sublatice. Chem. Mater. 27:3280–3290.
5. M Sturza, C D Malliakas, D E Bugaris, F Han, D Y Chung and M G Kanatzidis (2014) $NaCu_6Se_4$: A layered compound with mixed valency and metallic properties, Inorg. Chem. 53(22):12191-12198.

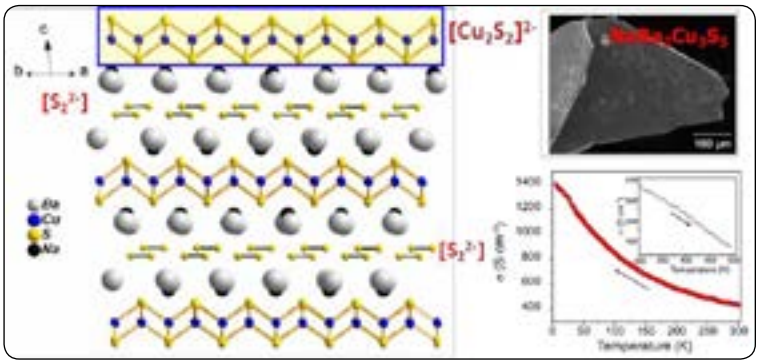

Figure 1: Crystal structure, SEM image and conductivity measurement of $NaBa_2Cu_3S_5$ crystal, a novel mixed-valent transition metal chalcogenide discovered by polychalcogenide flux synthesis.

Biography

Mihai I Sturza has his expertise in synthesis and crystal structure characterization of novel inorganic compounds. The main aim of his work is to synthesize new inorganic compounds (new oxides, oxo-halides, pnictides, chalcogenides, intermetallics, etc.) and to correlate their chemical and physical properties to their compositions and crystal structures. His research at IFW involves searching for novel low-dimensional materials with interesting electronic properties emerging from a competition between different electronic states or a suppression of the electronic order (charge, orbital or spin).

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