NEW COPPER CHALCOGENIDES WITH MIXED VALENCE

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9.7 cm

We perform a comparative study of several new ternary copper chalcogenides with alkali metals and rare earth elements, synthesized recently. We focus on their electronic, magnetic and transport properties as well as the lattice structures. It turns out that in majority of these systems it is not copper but chalcogen which is mixed valent and the charge transport as well as charge orderings are dominated by the p-ligand holes. The most striking and unique features of these materials are: 1) The unusual linear in T behavior of metallic resistivity up to $T \ll \Theta_D$ found in $K_3Cu_8Te_6$, $KCu_{7-x}S_4$, $La_2CuS_{4-\delta}$ and $Y_2Cu_2S_{5-\delta}$, being similar to that observed in high-T_c oxides. 2) The occurrence of untypical metal-nonmetal transitions at T_M - in $K_3Cu_8Se_6$ ($T_M \sim 160^oK$), $BaCuS_{3-x}$ ($\sim 270^oK$), $K_3Cu_8Se_6$ ($\sim 100^oK$), $TlCu_{7-x}S_4$ ($\sim 180^oK$), $KCu_{7-x}S_4$ ($\sim 190^oK$) with, surprisingly, low temperature phases being metallic, while the high-temperature ones– semiconducting. 3) Phase transitions connected with CDW formation - in $K_3Cu_8S_6$, $RbCu_8S_6$, and $K_3Cu_8Se_6$.
Electronic structure of the systems studied is discussed as a function of the charge transfer energy, the d-d Coulomb repulsion and the anion bandwidth.

13.4 cm

Subject category :

3. Transition Metals, Alloys and Compounds

Presentation mode :
poster

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