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Temperature-dependent behavior of mixed-valent SmS : a DFT+DMFT study CHANG-JONG KANG[1], HONG CHUL CHOI, KYOO KIM, B. I. MIN, Pohang University of Science and Technology (POSTECH) — We have investigated temperature-dependent behaviors of electronic structure and resistivity in a mixed-valent golden phase of SmS (g-SmS), based on the dynamical mean-field theory band structure calculations. Upon cooling, the coherent Sm 4f bands are formed to produce the hybridization-induced pseudo-gap near the Fermi level, and accordingly the topology of Fermi surface is changed. Also we have discussed the topological nature in g-SmS. From the analysis of anomalous resistivity behavior in SmS, we have identified universal energy scales, which characterize the Kondo/mixed-valent semimetallic systems.

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