

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Reduced Influence of Electronic Correlations in a Half-Filled System: Metallic Properties and Charge Order Transition in κ -(ET)₂Hg(SCN)₂Cl¹ NATALIA DRICHKO, Johns Hopkins University, REBECCA BEYER, MARTIN DRESSEL, University Stuttgart, Germany, HARALD JESCHKE, University Frankfurt, Germany, JOHN SCHLUETER, Argonne National Laboratory, ELENA ZHILYAEVA, RIMMA LYUBOVSKAYA, Institute of Problems of Chemical Physics, Russia — The family of κ -(ET)₂Hg(SCN)_xCl_{2-x} can be described within a model of a metal with a half-filled conductance band. Our calculations indicate that the value of the on-site Coulomb repulsion U is relatively small in these system. We investigate the effects of lower U on the optical properties of κ -(ET)₂Hg(SCN)₂Cl in the metallic state and below the metal-insulator transition. Optical conductivity spectra in the metallic state above 35 K show a behavior already observed for half-filled metals on the edge of the Mott insulating state: an optical transition between Hubbard bands at frequencies equal to U is present in spectra at all temperatures, being a precursor of a Mott transition, while a coherent carriers response develops below $T^*=150$ K. We note an influence of the lower U value both on the position of the “ U -band” and on a relatively high T^* . Untypically for a half-filled system, a metal-insulator transition at 35 K is found that is of a charge-order nature. A possibility of a charge-order ground state in a half-filled system in case of low U and relatively high nearest-neighbor Coulomb repulsion V is discussed.

¹Supported by H. Blewett fellowship

Natalia Drichko
Johns Hopkins University

Date submitted: 09 Dec 2011

Electronic form version 1.4