Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Structural and Electronic properties of the 2D Superconductor CuS covellite with 113-valent Copper IGOR MAZIN, Naval Research Laboratory — Hexagonal CuS has recently been reported to superconduct at 40 K. At the same time, earlier experiments had found superconductivity at 1.5 K. Some authors reported local magnetic moments in this compound, while others observe pure Pauli paramagnetism. It exhibits a rather unusual for a good metal symmetry-lowering transition at 55 K of unknown origin. Even the Cu valency in CuS has been debated, with suggested ionic models such as $(Cu^{+1})_3(S_2^{-2})(S^{-1})$ and $(Cu^{+1})_3(S_2^{-1})(S^{-2})$, as well as noninteger valencies. To gain more insight, we've performed DFT calculations and found that the actual valency of Cu is 4/3 (2), so that the Cu d band is not sufficiently ionized in the ideal compound to provide enough proximity to Mott dielectric for either local moments or unconventional superconductivity. On the other hand, the reason that Cu in not divalent here is that some sulfurs form covalent S_2 molecules with the effective S_2^{-2} valency. If some of these covalent S-S bonds are broken, local moments *can* form, and in that case superexchange in the hexagonal lattice can induce $f-$wave pairing. Finally, regarding the structural transition, it is well reproduced in DFT calculations. Possible microscopic origin of this transition will be discussed in the talk.

Igor Mazin
Naval Research Laboratory

Date submitted: 04 Nov 2011 Electronic form version 1.4