

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Novel Phase Between Band and Mott Insulators in Two Dimensions¹ SRIVENKATESWARA SARMA KANCHARLA, Oak Ridge National Laboratory, Materials Science and Technology Division, ELBIO DAGOTTO, Oak Ridge National Laboratory, Materials Science and Technology Division and University of Tennessee, Knoxville — We investigate the ground state phase diagram of the half-filled repulsive Hubbard model in two dimensions in the presence of a staggered potential Δ , the so-called ionic Hubbard model, using cluster dynamical mean field theory. We find that for large Coulomb repulsion, $U \gg \Delta$, the system is a Mott insulator (MI). For weak to intermediate values of Δ , on decreasing U , the Mott gap closes at a critical value $U_{c1}(\Delta)$ beyond which a correlated insulating phase suggesting bond order (BO) is found. Further, this phase undergoes a first-order transition to a band insulator (BI) at $U_{c2}(\Delta)$ with a finite charge gap at the transition. For large Δ , there is a direct first-order transition from a MI to a BI with a single metallic point at the phase boundary.

¹S.S.K. is supported by the LDRD program at Oak Ridge National Laboratory. E.D. acknowledges support by the NSF Grant No. DMR-0454504.

Srivenkateswara Sarma Kancharla
Oak Ridge National Laboratory

Date submitted: 29 Nov 2006

Electronic form version 1.4