Novel Phase Between Band and Mott Insulators in Two Dimensions[1] 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, $U >> \Delta$, 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.

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