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Abstract for an Invited Paper
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Formal Valence, $3d$ Occupation, and Charge Ordering Transitions[1]

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The metal-insulator transition (MIT), discovered by Verwey in the late 1930s, has been thought to be one of the best understood of MITs, the other ones being named after Wigner, Peierls, Mott, and Anderson. Continuing work on these transitions finds in some cases less and less charge to order, raising the fundamental question of just where the entropy is coming from, and just what is ordering. To provide insight into the mechanism of charge-ordering transitions, which conventionally are pictured as a disproportionation, I will (1) review and reconsider the charge state (or oxidation number) picture itself, (2) introduce new theoretical results for the rare earth nickelates (viz. $YNiO_3$), the putative charge ordering compound $AgNiO_2$, and the dual charge state insulator AgO, and (3) analyze cationic occupations of actual (not formal) charge, and work to reconcile the conundrums that arise. Several of the clearest cases of charge ordering transitions involve no disproportion; moreover, the experimental data used to support charge ordering can be accounted for within density functional based calculations that contain no charge transfer The challenge of modeling charge ordering transitions with model Hamiltonians will be discussed.

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