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Wannier function analysis of charge states in transition metal oxides[1] YUNDI QUAN, WARREN PICKETT, Univ of California - Davis — The charge (or oxidation) state of a cation has been a crucial concept in analyzing the electronic and magnetic properties of oxides as well as interpreting "charge ordering" metal-insulator transitions. In recent years a few methods have been proposed for the objective identification of charge states, beyond the conventional (and occasionally subjective) use of projected densities of states, weighted band structures (fatbands), and Born effective charges. In the past two decades Wannier functions (WFs) and particularly maximally localized WFs (MLWFs), have become an indispensable tool for several different purposes in electronic structure studies. These developments have motivated us to explore the charge state picture from the perspective of MLWFs. We will illustrate with a few transition metal oxide examples such as AgO and YNiO3 that the shape, extent, and location of the charge centers of the MLWFs provide insights into how cation-oxygen hybridization determines chemical bonding, charge distribution, and "charge ordering."

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