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Characterizing Oxidation State using Bader Analysis, Maximally Localized Wannier Functions and Atomic Orbitals Projection KYLE REEVES, YOSUKE KANAI, University of North Carolina at Chapel Hill — The concept of oxidation state of atoms in molecules and materials is widely used to predict and understand chemical and physical properties. This concept is perhaps driven more empirically than by any rigorous criteria differentiating one oxidation state from another. Within the oxidation state framework, an integer number of electrons is assigned to the nuclei within a system. In practice, a distribution of electron density makes it difficult to quantify such discrete assignments without some ambiguities. We explore three different charge analysis approaches in density functional theory calculations for addressing the oxidation state of important organometallic molecules $[Ru(bpy)_3]^{2+}$ and $[Ru(bpy)_3]^{3+}$, which are widely used for solar energy conversion applications. Bader charge analysis, Wannier function analysis, and atomic orbital projection are employed in this work. Given the highly-localized nature of the d-electrons of the ruthenium atom, the charge analysis methods are also compared with Hubbard-U correction. We also discuss how the solvation by water molecules influences the oxidation state characterization for these organometallic complexes.

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