The SCAN Density Functional: Predictive Power of 17 Exact Constraints*

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Kohn-Sham density functional theory in principle predicts the exact ground-state energy and electron density of a many-electron system via the solution of self-consistent one-electron Schrödinger equations. Only the exchange-correlation energy as a functional of the density needs to be approximated. For materials discovery, the approximations need to be computationally efficient, predictive, and usefully accurate. The SCAN (strongly constrained and appropriately normed) meta-generalized gradient approximation was constructed [1] to satisfy all 17 known exact constraints that a semi-local functional can satisfy (compared to 11 for the PBE GGA). SCAN is further fitted to appropriate norms, non-bonded systems for which a semi-local functional can be accurate for exchange and correlation separately. SCAN recognizes and provides different GGA-like descriptions for covalent single bonds, metallic bonds, and van der Waals (vdW) bonds. Here I will review the functional itself, along with its long-range vdW extension SCAN+rVV10 [2]. I will also review applications to properties of diversely-bonded systems [3], including ferroelectricity [4], density and structure of liquid water [5], crystal structure stability [6], surface properties of transition metals [7], and critical pressures for structural phase transitions of semiconductors [8]. The accuracy of SCAN is often comparable to or better than that of a hybrid functional, at lower computational cost and without any fitting to bonded systems.

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