

# Localized Orbital Scaling Correction for Systematic Elimination of Delocalization Error in Density Functional Approximations

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## **Abstract**

The delocalization error of popular density functional approximations (DFAs) leads to diversified problems in present-day density functional theory calculations. For achieving a universal elimination of delocalization error, we develop a localized orbital scaling correction (LOSC) framework, which unifies our previously proposed global and local scaling approaches. The LOSC framework accurately characterizes the distributions of global and local fractional electrons, and is thus capable of correcting system energy, energy derivative and electron density in a self-consistent and size-consistent manner. The LOSC-DFAs lead to systematically improved results, including the dissociation of cationic species, the band gaps of molecules and polymer chains, the energy and density changes upon electron addition and removal, and photoemission spectra.

## **Reference**

Chen Li, Xiao Zheng, Neil Qiang Su, Weitao Yang; Localized orbital scaling correction for systematic elimination of delocalization error in density functional approximations, National Science Review, nwx111, <https://doi.org/10.1093/nsr/nwx111>