# Estimation of the Effective On-Site Coulomb Interaction Parameter U by Mapping Atomic Self-Interaction Correction onto GGA+U for Molecules

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It is known that the on-site Coulomb interaction parameter, also called as the Hubbard U parameter, can be obtained from a density functional theory (DFT) linear-response method [1], but this approach is not available to DFT calculation on atom-centered basis sets because density response to a localized potential shift cannot be described due to the unclear definition of the Hubbard U values for multiple-zeta orbitals and the limit of accuracy reinforcement by increasing the number of basis functions.

I propose a calculation method for effective on-site interaction U parameters by taking advantage of the relationship between GGA+U (or LDA+U) and atomic self-interaction correction (ASIC) [2]. Because molecular orbitals containing transition metal 3*d* orbitals are often close to atomic-like orbitals, the unitary matrix (transformation between Kohn-Sham orbitals and so-called ‘localized orbitals’) elements related with the 3*d* orbitals can be assumed to be square-roots of the Mulliken 3*d* orbital populations for molecular orbitals. From the specific unitary matrix elements, one can obtain the localized orbitals corresponding to the 3*d* orbitals, which can give effective U values.

Calculated effective U values were reasonable for simple molecules containing a transition metal atom when a numerical atomic orbital code package, OpenMX was used with dual projectors [3]. My results are comparable to the results of the linear-response method on plane-wave basis sets.

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