Ab initio study of chromium isotopes

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Density functional theory (DFT) is widely used in solid state physics and chemistry. However, there is no self-interaction error-free functionals available so far. Here, we are going to introduce Fermi-Löwdin-orbital self-interaction corrected DFT and its application on the studies of chromium isotopic system, an important tracer of free oxygen and biostimulated activities.