# Open source code development for DFT + DMFT calculation: correlated subspace projection and analytic continuation

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In the strongly correlated electron systems, it is crucial to provide an appropriate theoretical formalism that can handle many-body effects in a material-specific context. One of the successful approaches is the dynamical mean-field theory (DMFT) combined with the DFT [1]. We implemented DFT+DMFT based on OpenMX, a pseudo-atomic orbital basis DFT code [2]. The implementation is characterized as follows: i) the wide energy window on which the hybridization function is defined, including ligand orbitals, e.g., oxygen *p* orbitals. ii) projection method that defines correlated subspace based on the natural atomic orbitals (NAOs) [3]. With this NAOs-based projector, *d*-*p* hybridization can be reasonably described. We also discuss the newly developed methods for analytic continuation problem, the so-called maximum quantum entropy method (MQEM) [4]. We show that the results are stable for numerical parameter changes, applying our methods to the typical transition metal oxide systems.

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