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DMFTwDFT: An open-source code combining Dynamical Mean Field Theory with various Density Functional Theory packages[1] UTHPALA HERATH, Department of Physics and Astronomy, West Virginia University, VIJAY SINGH, BENNY WAH, XINGYU LIAO, Department of Physics, University of Illinois at Chicago, ALDO ROMERO, Department of Physics and Astronomy, West Virginia University, HYOWON PARK, Department of Physics, University of Illinois at Chicago, UNIVERSITY OF ILLINOIS AT CHICAGO COLLABORATION, WEST VIRGINIA UNIVERSITY COLLABORATION — Dynamical Mean Field Theory (DMFT) is a successful method to compute the electronic structure of strongly correlated materials, especially when it is combined with density functional theory (DFT). Here, we present an open-source computational package (and a library) combining DMFT with various DFT codes interfaced through the Wannier90 package. The correlated subspace is expanded as a linear combination of Wannier functions introduced in the DMFT approach as local orbitals. In particular, we provide a library mode for computing the DMFT density matrix. This library can be linked and then internally called from any DFT package, assuming that a set of localized orbitals can be generated in the correlated subspace. The existence of this library allows developers of other DFT codes to interface with our package and achieve the charge-self-consistency within DFT+DMFT loops. To test and check our implementation, we computed the density of states and the band structure of well-known correlated materials, namely $LaNiO_3$, $SrVO_3$, and NiO. The obtained results are compared to those obtained from other DFT+DMFT implementations.

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Uthpala Herath
Department of Physics and Astronomy, West Virginia University

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