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Hellmann-Feynman Forces within the DFT+U in Wannier functions basis DMITRY NOVOSELOV, DMITRY KOROTIN, VLADIMIR ANISIMOV, Institute of Metal Physics — The most general way to describe localized atomic-like electronic states in strongly correlated materials is to use Wannier functions. In the present paper we continue development of widely-used DFT+U method with the Wannier function basis set and propose a technique to calculate Hubbard contribution to atomic forces. The technique was implemented as a part of plane-waves pseudopotential code Quantum-ESPRESSO and tested on two compounds: charge transfer insulator NiO with cubic crystal structure and correlated metal $SrVO_3$ with perovskite structure.

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