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**Ultrasoft pseudopotentials and Hubbard U values for rare-earth elements (Re=La-Lu) guided by HSE06 calculations** MEHMET TOPSAKAL, KOICHIRO UMEMOTO, RENATA WENTZCOVITCH, University of Minnesota — The lanthanide series of the periodic table comprises fifteen members ranging from La to Lu - the rare-earth (Re) elements. They exhibit unique (and mostly unexplored) chemical properties depending on the fillings of 4f-orbitals. Due to strong electronic correlation, 4f valence electrons are incorrectly described by standard DFT functionals. In order to cope with these inefficiencies, the DFT+U method is often employed where Hubbard-type U is introduced into the standard DFT. Another approach is to use hybrid functionals. Both improve the treatment of strongly correlated electrons. However, DFT+U suffers from ambiguity of U while hybrid functionals suffer from extremely demanding computational costs. Here we provide Vanderbilt type ultrasoft pseudopotentials for Re elements with suggested U values allowing efficient plane-wave calculations. Hubbard U values are determined according to HSE06 calculations on Re-nitrides (ReN). Generated pseudopotentials were further tested on some Re-cobaltite (Re-CoO3) perovskites. Alternative pseudopotentials with f-electrons kept frozen in the core of pseudopotential are also provided and possible outcomes are addressed. We believe that these new pseudopotentials with suggested U values will allow further studies on rare-earth materials.

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