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Importance of the $5f$-Pseudopotential for $5d$ Transition Metals NICHOLS ROMERO, University of Illinois at Urbana-Champaign, NITHAYA CHETTY, University of KwaZulu-Natal, Pietermaritzburg, RICHARD MARTIN, University of Illinois at Urbana-Champaign — It is usual to neglect the $\ell = 3$ component of the pseudopotential (PP) in *ab initio* density functional calculations of $5d$ transition metals. In most of these elements, the $5f$ orbitals are unbound in the neutral ground-state configuration of the atom. We construct the $5f$-PP using the Hamman procedure for unbound states [1], and carry out planewave (PW) calculations using ABINIT [2] for selected $5d$ transition metals. We show that omission of the $5f$-PP leads to systematic errors in the bulk properties for some elements. Although all-electron (AE) methods are often used for studying these materials in bulk, the PP-PW method is computational less expensive by comparison and can be readily used to study complicated geometries like surfaces. The $5d$ transition metals are important elements because they form stable hard materials. For example, iridium is used in the calibration of high pressure diamond anvils because of its extreme stability at high pressure and temperature. [1] D. R. Hamann, Phys. Rev. B 40 2980 (1989). [2] X. Gonze et. al, Comp. Mat. Sci. 25, 478 (2002).

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