Pseudopotentials for first-principles calculations of uranium compounds

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The pseudopotential approach allows reducing the total number of electrons in the model that speeds up calculations. However, there is a lack of pseudopotentials for heavy elements suitable for condensed matter DFT models. In this work, we present a pseudopotential for uranium developed in the Goedecker-Teter-Hutter form. Its accuracy is illustrated using several molecular and solid-state calculations.