Abstract Submitted
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Optimization Algorithm for the Generation of ONCV Pseudopotentials[1] MARTIN SCHLIPF, FRANCOIS GYGI, Univ of California - Davis — We present an optimization algorithm to construct pseudopotentials and use it to generate a set of Optimized Norm-Conserving Vanderbilt (ONCV) pseudopotentials[1] for elements up to Z=83 (Bi) (excluding Lanthanides). We introduce a quality function that assesses the agreement of a pseudopotential calculation with all-electron FLAPW results, and the necessary plane-wave energy cutoff. This quality function allows us to use a Nelder-Mead optimization algorithm on a training set of materials to optimize the input parameters of the pseudopotential construction for most of the periodic table. We control the accuracy of the resulting pseudopotentials on a test set of materials independent of the training set. We find that the automatically constructed pseudopotentials provide a good agreement with the all-electron results obtained using the FLEUR code [2] with a plane-wave energy cutoff of approximately 60 Ry.
[1] D. R. Hamann, Phys. Rev. **B88**, 085117 (2013).
[2] FLEUR code, http://www.flapw.de

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