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A new type of pseudopotentials: effective atomic pseudopotentials JAIRO RICARDO CARDENAS, ROBY CHERIAN, GABRIEL BESTER, Max Planck Institute for Solid State Research — We derive a new type of pseudopotentials from conventional norm-conserving pseudopotentials for the treatment of a large number of atoms. The pseudopotentials are not aimed at the calculation of the total energy, but of band edge states relevant for optical processes. We describe the pseudopotential construction and benchmark its quality and transferability by comparison to standard DFT calculations.

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