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Real-space pseudopotential method for noncollinear magnetism within density functional theory DORON NAVEH, LEEOR KRONIK, Weizmann Institute of Science, Israel — We present a real-space pseudopotential method for first principles calculations of noncollinear magnetic phenomena within density functional theory. We demonstrate the validity of the method using the test cases of the Cr_3 the a Cr monolayer. The approach retains all the typical benefits of the real-space approach, notably massive parallelization. It can be employed with arbitrary boundary conditions and can be combined with the computation of pseudopotential-based spin-orbit coupling effects.

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