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Ab initio calculation of the orbital magnetization by Wannier interpolation GRAHAM LOPEZ, Wake Forest University, DAVID VANDERBILT, Rutgers University, IVO SOUZA, University of California Berkeley, TIMO THONHAUSER, Wake Forest University — We present an analytic, first-principles scheme to efficiently calculate exactly the spontaneous orbital magnetization of ferromagnetic crystals [1,2]. This is in contrast to the standard method of integrating inside muffin-tin spheres which, while a good approximation in practice, is still an approximation. The method uses Wannier interpolation to perform the necessary Brillouin-zone integrals in a similar way as was done previously for the anomalous Hall conductivity [3]. The method has been implemented to work with a plane-wave density-functional code, and calculations were done on iron, cobalt and nickel. We compare our calculations of the orbital magnetization in these systems to recent ab initio and experimental results and find good agreement with both [4].

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