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Orbital magnetization in a supercell framework: Single k-point formula DAVIDE CERESOLI, SISSA and Democritos National Simulation Center, Trieste, RAFFAELE RESTA, University of Trieste and Democritos National Simulation Center, Trieste — The position operator **r** is ill-defined within periodic boundary conditions: owing to this, both the macroscopic (electric) polarization and the macroscopic orbital magnetization are nontrivial quantities. While the former has been successfully tamed since the early 1990s, the latter remained a long-standing unsolved problem. A successful formula within DFT for crystalline systems has been recently found.[1] The formula is based on a Brillouin-zone integration, which is discretized on a reciprocal-space mesh for numerical implementation. We find here the single **k**-point limit, useful for large enough supercells, and particularly in the framework of Car-Parrinello simulations for noncrystalline systems. We validate our formula on the test case of a crystalline system, where the supercell is chosen as a large multiple of the elementary cell. Rather counterintuitively, even the Chern number (in 2d) can be evaluated using a single **k**-point diagonalization.

[1]D. Ceresoli, T. Thonhauser, D. Vanderbilt, R. Resta, Phys. Rev. B **74**, 024408 (2006).

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