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The magnetization of periodic solids from time-dependent current-density-functional theory ARJAN BERGER, Laboratoire de Chimie et Physique Quantiques (LCPQ), Universite Paul Sabatier, Toulouse, France and European Theoretical Spectroscopy Facility (ETSF), NATHANIEL RAIMBAULT, Laboratoire de Chimie et Physique Quantiques (LCPQ) and Laboratoire de Physique Théorique (LPT), Université Paul Sabatier, Toulouse, France, PAUL DE BOEIJ, Scientific Computing & Modelling (SCM), Amsterdam, The Netherlands, PINA ROMANIELLO, Laboratoire de Physique Théorique (LPT), Université Paul Sabatier, Toulouse, France and European Theoretical Spectroscopy Facility (ETSF) — The evaluation of the macroscopic magnetization of solids is problematic when periodic boundary conditions are used because surface effects are artificially removed. This poses a problem unless surface effects can be reformulated in terms of bulk quantities. For example, in case of the macroscopic polarization one can express the contribution of the charge density accumulated at the surface in terms of the bulk current density through the continuity equation. Therefore one can work in the framework of time-dependent current-density functional theory to efficiently calculate the macroscopic polarization [1,2]. In this presentation we will show how also the magnetization can be described within this framework.

[1] F. Kootstra, P. L. de Boeij, and J. G. Snijders, J. Chem. Phys. 112, 6517 (2000).
[2] J. A. Berger, P. Romaniello, R. van Leeuwen, and P. L. de Boeij , Phys. Rev. B 74, 245117 (2006)

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