

Abstract Submitted
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Advances in time-dependent current-density functional theory¹

ARJAN BERGER, University of Toulouse III - Paul Sabatier — In this work we solve the problem of the gauge dependence of molecular magnetic properties (magnetizabilities, circular dichroism) using time-dependent current-density functional theory [1]. We also present a new functional that accurately describes the optical absorption spectra of insulators, semiconductors and metals [2]

N. Raimbault, P.L. de Boeij, P. Romaniello, and J.A. Berger Phys. Rev. Lett. 114, 066404 (2015)

J.A. Berger, Phys. Rev. Lett. 115, 137402 (2015)

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