

Abstract Submitted
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Gauge invariant calculation of magnetic properties from time-dependent current DFT¹ NATHANIEL RAIMBAULT, Laboratoire de Chimie et Physique Quantiques, IRSAMC, Université Toulouse III - Paul Sabatier, CNRS & European Theoretical Spectroscopy Facility, PAUL L. DE BOEIJ, Scientific Computing & Modeling NV, Vrije Universiteit, Theoretical Chemistry, PINA ROMANIELLO, Laboratoire de Physique Théorique, CNRS, IRSAMC, Université Toulouse III - Paul Sabatier & European Theoretical Spectroscopy Facility, ARJAN BERGER, Laboratoire de Chimie et Physique Quantiques, IRSAMC, Université Toulouse III - Paul Sabatier, CNRS & European Theoretical Spectroscopy Facility — We present a method to calculate magnetic properties from the current density that does not depend on the gauge choice for the vector potential when a finite basis set is used [1]. To obtain this we put paramagnetic and diamagnetic contributions to the current on equal footing by making use of a sum rule [1]. Our method is general. Here we use it to calculate static and dynamical magnetizabilities of molecules within Time-Dependent Current-Density-Functional Theory.

[1] N. Raimbault, P.L. de Boeij, P. Romaniello, and J.A. Berger, submitted

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