Gauge invariant calculation of magnetic properties from time-dependent current DFT\(^1\) 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.

\[^1\] This study has been partially supported through the grant NEXT ANR-10-LABX-0037 in the framework of the Programme des Investissements d’Avenir.

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Date submitted: 13 Nov 2014

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