

Abstract Submitted
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Optical and magnetic excitations in small transition-metal clusters using TDDFT¹ MICAEL OLIVEIRA, FERNANDO NOGUEIRA, Center for Computational Physics, University of Coimbra, Portugal, ANGEL RUBIO, Facultad de Químicas, Universidad del País Vasco, Spain — Magnetic properties of transition-metal clusters have been the subject of intensive study in the last decades both theoretical and experimentally. In particular, the importance of noncollinear effects and spin-orbit coupling in those systems has recently gained great interest. In this work we use time dependent density functional theory (TDDFT) to study optical and magnetic excitations of small transition-metal clusters. In particular, we investigate the role of non-collinear magnetism and spin-orbit coupling in such phenomena. We present some results concerning the linear response calculations and show how noncollinear effects and spin-orbit coupling modify the optical and/or magnetic spectra (including the natural magnetic dichroism spectroscopy). We will discuss further line of research that we are conducting to understand the size dependence magnetic response of this clusters for potential technological applications. The calculations are done within a real-time real-space TDDFT framework using the Octopus code.

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