DFT STUDY ON A CHAIN MODEL OF THE CHROMIUM-BASED MOLECULAR MAGNETS

D. M. Tomecka\textsuperscript{1,2}, V. Bellini\textsuperscript{2}, F. Troiani\textsuperscript{2}, F. Manghi\textsuperscript{2}, G. Kamieniarz\textsuperscript{1}, and M. A®ronte\textsuperscript{2}

\textsuperscript{1}Computational Physics Division, Institute of Physics, A. Mickiewicz University, Poznaï, Poland
\textsuperscript{2}CNR-INFM-S3 and Department of Physics, University of Modena and Reggio Emilia, Modena, Italy

We present a density functional theory (DFT) study of the electronic and magnetic properties of the chromium-based molecular rings. The all-electron linearized augmented plane wave method (LAPW) implemented in the Wien2k package \cite{1} is used to calculate the electronic states, exchange coupling parameters and magnetic anisotropy of an infinite chain model system of Cr\textsubscript{8}. We demonstrate how the chain model mimics with good approximation the electronic and magnetic properties of the original Cr\textsubscript{8} molecule \cite{2}, and offers an unique opportunity, in virtue of the reduced computational effort, for carrying out extensive investigations of molecules belonging to the Cr-based molecular rings family \cite{3}.

\begin{itemize}
  \item \cite{1} P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka, and J. Luitz, WIEN2K, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties (see www.wien2k.at for details).
  \item \cite{3} D. M. Tomecka, V. Bellini, F. Troiani, F. Manghi, G. Kamieniarz, and M. A®ronte (to be submitted).
\end{itemize}

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Corresponding author : D.M. Tomecka

Address for correspondence : Umultowska 85
64-614 Poznaï
Poland

Email address : tomecka@amu.edu.pl