Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Development in the DFT estimates of magnetic couplings in chromium-based molecular rings from an optimally-tuned range separated hybrid functional SHIRA WEISSMAN, Weizmann Institute of Science, Israel, MICHAŁ ANTKOWIAK, GRZEGORZ KAMIENIARZ, A. Mickiewicz University, Poland, LEEOR KRONIK, Weizmann Institute of Science, Israel — The Cr_8 molecule, as well as its homo- and hetero-metallic derivatives, belongs to a class of molecular nanomagnets which are extensively studied for a number of fundamental aspects and envisaged applications. However, estimating accurately their magnetic couplings from first principles calculations has proven to be difficult. Here we present progress in this area for two prototypical molecular rings, Cr_8 and Cr_7Ni^-, using density functional theory with an optimally-tuned range separated hybrid (OT-RSH) functional. This approach has been shown to allow for an accurate description of the electronic structure in a variety of more simple molecular systems. Here, we show that it is also capable of producing highly accurate magnetic exchange parameters for both molecules despite their complexity, while improving the overall description of the electronic structure, especially with respect to the energy of the frontier orbitals. For the Cr_7Ni^- ring, the values of the magnetic couplings found are distinguished by a unique site distribution and lead to excellent agreement with experiment.

Shira Vaisman
Weizmann Institute of Science

Date submitted: 09 Nov 2016 Electronic form version 1.4