

# DFT augmented symmetry approach applications to simulations of the chromium-based rings: cross-validation using the PBE and B3LYP functionals

Michał Wojciechowski,<sup>1</sup> Bartosz Brzostowski,<sup>1</sup> and Grzegorz Kamieniarz<sup>2</sup>

<sup>1</sup>*Institute of Physics, University of Zielona Góra, Poland*

<sup>2</sup>*Faculty of Physics, A. Mickiewicz University, Poznań, Poland*

The DFT estimates of magnetic couplings in molecular nanomagnets are computationally demanding and their values have not achieved the satisfactory accuracy in spite of a lot of effort. We concentrate here on comprehensive convergence and accuracy tests for predictions of the augmented symmetry approach aiming at reducing the computational complexity of the DFT calculations for molecular rings which is particularly important for the Wien2k code. Using both the PBE and the B3LYP functionals, we demonstrate the numerical stability of magnetic couplings, magnetic moments and the HOMO-LUMO gaps, changing the size of the basic parameters RKM, the number of k-points and types of the unit cells as well as some symmetry constraints. We reach the significant gain in the computing time without a loss in the accuracy of the final results with respect to those obtained by the standard approaches which paves the way to application of the hybrid functionals within Wien2k. We conclude that the value  $RKM = 3.0$  and a single k-point in the irreducible Brillouin zone are enough for estimation of magnetic couplings.