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Anisotropy, geometric structure and frustration effects in molecule-based nanomagnets

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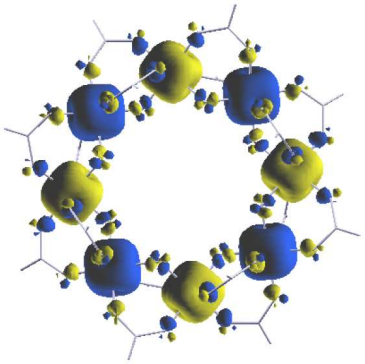
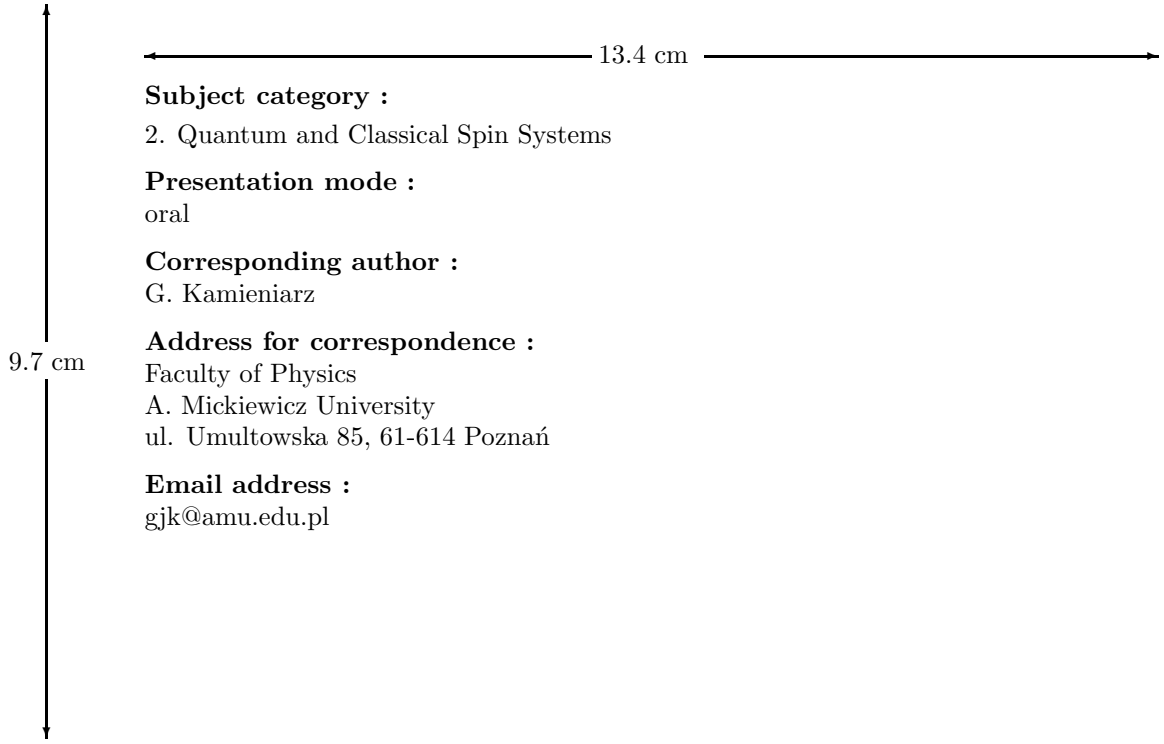


Molecular nanomagnets are based on transition metal ions, which determine their magnetic properties. Magnetic shielding of the molecules by organic ligands allows the quantum effects characteristic of a single molecule to be measured in a bulk sample. In view of possible applications, precise modeling of such materials plays a very important role. In the lecture we are going to present results on anisotropy, geometric structure and frustration effects in a family of molecular rings and chains obtained by means of various complementary numerical simulations both phenomenological and ab-initio. The precise numerical results obtained can be used to test theoretical models or as guidelines for experiment.

The chromium-based molecular ring $Cr_8F_8Piv_{16}$ (abbreviated as Cr_8) is a precursor of a family of chromium nano-rings. The localization of the spin density on Cr(III) ions is shown in Figure. The Cr_7Cd complex is another member of the family. It was obtained by substituting one of the chromium centers in Cr8 with a non-magnetic Cd ion. We assume that these compounds can be modeled by the anisotropic Heisenberg Hamiltonian which yields a very good fit to susceptibility and magnetization. It is demonstrated that the best results in modeling magnetic torque of Cr_7Cd can be obtained by taking into account bond dependent exchange anisotropy. Another interesting property analyzed was magnetic frustration in a model of nine-membered chromium ring (Cr_9) with a bond defect. We specified local and global thermodynamic quantities which can serve as frustration signatures and showed how frustration depends on the magnitude of a bond defect.

The magnetic properties of the bimetallic zig-zag shaped chains with Re(IV) and Cu(II) complexes were numerically analyzed on the basis of the planar model which takes into account the site-dependent alternating directions of the local coordinate systems for the Re(IV) ions and the axial and rhombic single-ion anisotropy terms. A number of symmetries for the single-crystal susceptibility were found and the value of the rhombic anisotropy parameter accounting for some thermodynamic properties was estimated. The results of our simulations were successfully fitted to the corresponding experimental susceptibility data.



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