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EPR Spectroscopy of Manganese-Doped Perovskite-Type Metal-Organic Framework

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Recently, a new type of porous materials called coordination polymers or metal-organic frameworks (MOFs) emerged and attracted attention of the scientific community. These crystalline compounds are unique due to the highly porous structures which can be utilized for gas adsorption related applications. Some of MOF materials contain paramagnetic transition-metal ions, resulting in peculiar magnetic properties of these compounds. In addition, the organic part in some coordination polymers consists of polar molecules, which below a certain phase transition temperature order into a ferroelectric phase.
Lately, a promising MOF [(CH3)2NH2][Zn(HCOO)3] with perovskite-type architecture and inherent ferroelectricity was synthesized. It is believed that the ferroelectric phase in this material is due to the ordering of (CH3)2NH2+ ions, but, however, the precise phase transition mechanism is still obscure.
In this work we investigate the [(CH3)2NH2][Zn(HCOO)3] MOF doped with 0.05 mol% paramagnetic Mn2+ ions using the continuous-wave (CW) and pulsed EPR methods. The temperature dependent X-band CW and field-sweep as well as Q-band CW EPR spectra reveal that the local Mn2+ ion-probes are indeed sensitive to the local structural changes occurring at the phase transition point. Spectral simulations were used to obtain the g, hyperfine A and fine-structure D tensors and temperature dependence of their components allowing to further characterize the observed phase transition and the MOF structure. Following the temperature dependence of the axial zero-field splitting parameter D, it was concluded that the phase transition into the ferroelectric phase is of the first order.

Primary author: Mr SIMENAS, Mantas (Faculty of Physics, Vilnius University, Sauletekio av. 9, Vilnius, Lithuania LT-10222)

Co-authors: Prof. PÖPPL, Andreas (Faculty of Physics and Earth Sciences, Leipzig University, Linnestrasse 5, Leipzig, Germany D-04103); Prof. BANYS, Juras (Faculty of Physics, Vilnius University, Sauletekio av. 9, Vilnius, Lithuania LT-10222); Prof. MACZKA, Miroslaw (Institute of Low Temperature and Structure Research, Polish Academy of Sciences, 50-950 Wroclaw 2, Poland)

Presenter: Mr SIMENAS, Mantas (Faculty of Physics, Vilnius University, Sauletekio av. 9, Vilnius, Lithuania LT-10222)

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