THE 67TH INTERNATIONAL

OPEN READINGS

CONFERENCE FOR STUDENTS OF PHYSICS AND NATURAL SCIENCES

BOOK OF ABSTRACTS | 2024

Vilnius University

VILNIUS UNIVERSITY PRESS

Editors:

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Cover and Interior Design:

Goda Grybauskaitė

Vilnius University Press
9 Saulėtekio Av., III Building, LT-10222 Vilnius
info@leidykla.vu.lt, www.leidykla.vu.lt/en/
www.knygynas.vu.lt, www.journals.vu.lt

Bibliographic information is available
on the Lithuanian Integral Library Information System (LIBIS) portal www.ibiblioteka.lt
ISBN 978-609-07-1051-7 (PDF)

EPR SPECTROSCOPY OF STRUCTURAL PHASE TRANSITION IN $CH_3NH_3PbCl_3$ HYBRID PEROVSKITE

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Recently, hybrid organic-inorganic compounds have attracted immense attention of the scientific community due to their diverse physical and chemical properties. One of the most interesting and researched subgroups of hybrid perovskites is methylammonium (MA) lead halides $MAPbX_3$ (where X = I, Br, Cl), due to their potential applications in efficient and low-cost solar cells, LEDs, and photodetectors [1].

Here, we use electron paramagnetic resonance (EPR) spectroscopy to study the dynamics of methylammonium cations and structural phase transitions in methylammonium lead chloride $CH_3NH_3PbCl_3$. In this work, we employ temperature dependent multifrequency continious-wave (CW) and pulsed EPR spectroscopy to characterize paramagnetic Mn^{2+} probe ions in $MAPbX_3$. The temperature dependent CW spectra reveal a sudden increase in the zero-field splitting of the Mn^{2+} ions at about 175 K (Fig. 1). This indicates a first-order phase transition related to the deformation of the inorganic framework due to the tetragonal-orthorhombic symmetry lowering.

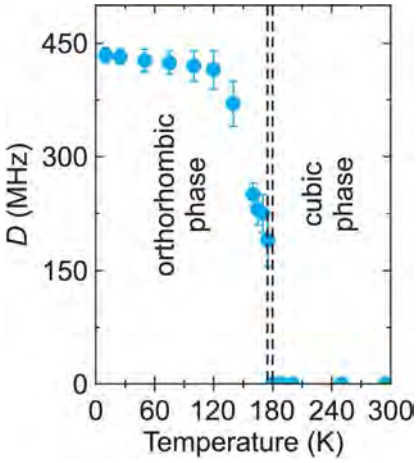

Fig. 1. Temperature dependence of the axial zero-field splitting parameter of $MAPbX_3$:Mn.

Using pulsed EPR spectroscopy, studying the temperature dependence of the T_1 relaxation time and the decoherence time T_2 of the Mn^{2+} centers in $MAPbCl_3$, we found that T_1 is governed by the direct process and the Raman process due to optical phonons. We relate the obtained phonon energy of 59(4) cm^{-1} to the dynamics of the inorganic framework.

This project has been funded by the Research Council of Lithuania (LMTLT) (agreement No. S-MIP-22-73).

[1] Kojima, A., et al., J. Am. Chem. Soc., 131, 6050-6051 (2009).