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Mn Antisites and Order-Disorder Transition in the (MnBi2Te4)(Bi2Te3)n Magnetic Topological Insulators

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Intrinsic magnetic topological insulators from the $MnBi_2Te_4$·$(Bi_2Te_3)_n$ family have garnered significant attention as versatile platforms capable of hosting a range of exotic quantum states and phenomena, including higher-order topological phases, axion electrodynamics, and the quantum anomalous Hall effect. This tunability arises from manganese–pnictogen intermixing, which is sensitive to synthesis conditions.
In this work [1], we use nuclear magnetic resonance and muon spin rotation and relaxation spectroscopy complemented by DFT calculations to explore the impact of the intermixing on the magnetic properties of (MnBi2Te4)(Bi2Te3)n and MnSb2Te4. Our findings show that Mn moments on native sites and antisites align oppositely in the ground state for $(MnBi_2Te_4)(Bi_2Te_3)_n$ (n = 0, 1, 2) and $MnSb_2Te_4$. Moreover, in all compounds, the Mn antisite sublattice disorders at temperatures significantly below the intrinsic magnetic transition, giving rise to an intermediate phase with a uniform magnetic structure unaffected by intermixing. This phase is likely where the anticipated exotic quantum states can be observed. Our results provide a microscopic understanding of the crucial role played by Mn-Bi intermixing and offer pathways for understanding the surface gap states.

Reference
[1] M. Sahoo, I. J. Onuorah et al., Adv. Sci., 11, 34, 2402753, 2024

Email

ifeanyijohn.onuorah@unipr.it

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Supervisors Name

Roberto De Renzi

Supervisors Email

roberto.derenzi@unipr.it

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Primary authors: ONUORAH, Ifeanyi John (Dipartimento di Scienze Matematiche Fisiche e Informatiche Universitá di Parma Parco delle Scienze 7A, Parma I-43124, Italy); SAHOO, Manaswini (Leibniz IFW Dresden Helmholtzstraße 20, D-01069 Dresden, Germany); FOLKERS, Laura Christina (Institut für Festkörper- und Materialphysik Technische Universität Dresden 01062 Dresden, Germany); KOCHETKOVA, Ekaterina (Van der Waals-Zeeman Institute Department of Physics and Astronomy University of Amsterdam Science Park 094, Amsterdam 1098 XH, Netherlands); CHULKOV, Evgueni V. (Donostia International Physics Center Sebastián 20018 Donostia-San, Spain); OTROKOV, Mikhail M. (Instituto de Nanociencia y Materiales de Aragón (INMA) CSIC-Universidad de Zaragoza Zaragoza 50009, Spain); ALIEV, Ziya S. (Baku State University Baku AZ1148, Azerbaijan); AMIRASLANOV, Imamaddin R. (Baku State University Baku AZ1148, Azerbaijan); WOLTER, Anja U. B. (Leibniz IFW Dresden Helmholtzstraße 20, D-01069 Dresden, Germany); BÜCHNER, Bernd (Leibniz IFW Dresden Helmholtzstraße 20, D-01069 Dresden, Germany); CORREDOR, Laura Teresa (Leibniz IFW Dresden Helmholtzstraße 20, D-01069 Dresden, Germany); WANG, Chennan (Laboratory for Muon Spin Spectroscopy Paul-Scherrer-Institute Villigen PSI CH-5232, Switzerland); SALMAN, Zaher (Laboratory for Muon Spin Spectroscopy Paul-Scherrer-Institute Villigen PSI CH-5232, Switzerland); ISAEVA, Anna (Leibniz IFW Dresden Helmholtzstraße 20, D-01069 Dresden, Germany); DE RENZI, Roberto (Department of Physics and Earth Sciences, University of Parma, IT-43124 Parma, Italy); ALLODI, Giuseppe (Dipartimento di Scienze Matematiche Fisiche e Informatiche Universitá di Parma Parco delle Scienze 7A, Parma I-43124, Italy)

Presenter: ONUORAH, Ifeanyi John (Dipartimento di Scienze Matematiche Fisiche e Informatiche Universitá di Parma Parco delle Scienze 7A, Parma I-43124, Italy)

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