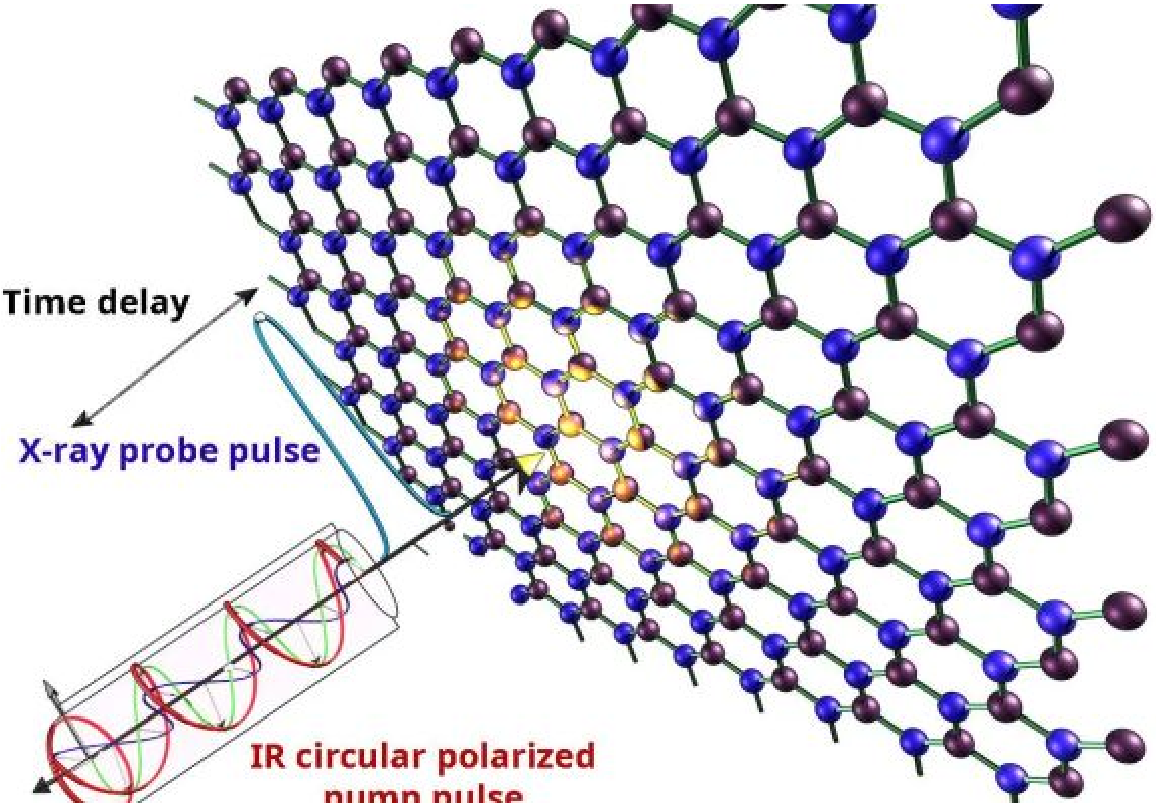

Tracing topological phase transitions with X-ray absorption techniques

An international team of researchers present in **Reports on Progress in Physics Original Research** a numerical experiment tha demonstrates the possibility to capture topological phas transitions via an x-ray absorption spectroscopy scheme. B overcoming previous energy resolution limitations, the metho will enable further investigations on relevant systems fo optoelectronics applications.

October 28, 2024

The atoms of solids, liquids, and gases exhibit very different arrangements and behavior. In solids, atoms are tightly packed in a regular pattern; in liquids, atoms are close together but randomly arranged and with some freedom to move; and in gases, atoms are further apart and can move freely. These features define the conventional phases of matter.

When one enters the quantum world, other phases of matter, which have nothing to do with atomic distribution or mobility, emerge. These are the **topological phases**. In this realm, some properties of the particles within a material (like atoms or electrons) can become connected through a phenomenon known as long-range entanglement. When a pair of particles is entangled, changing or measuring one of them immediately affects the other, regardless of the distance between them. These particles might be entangled in a complex pattern, spanning the entire system. Different ?entanglement patterns' of the material's electrons or other quantum particles define different topological phases. Thus, altering the way particle are entangled, rather than changing their spatial arrangement leads to a phase transition

Topological states of matter offer the potential to create exotic materials, which can be, fo instance, insulators in the bulk but hold conducting states on the surface. In the last years there has been enormous progress in the development of these modern materials. Fo example, some topologically non-trivial insulators could be induced by using ultrashor intense lasers. However, these light-induced topological insulators exist only while the lase pulse is on, that is, around several femtoseconds (10-15 seconds). This imposes a strong requirement to study and characterize them since an ultrafast probe in the femtosecond timescale is needed in order to capture the ultrafast topological phases.

Despite the significant progress in this direction, some challenges remain. For example, angle-resolved photoemission spectroscopy (ARPES) has proved to be effective in probing these topological systems, but it faces a drawback: the shorter the probe pulse duration (and, consequently, the closer for capturing the material's ultrafast nature), the lower the photoelectron energy resolution.

Recently, a team led by Universidad Autonoma de Madrid, with the collaboration of researchers from ICFO, **Dr. Emilio Pisanty**, **Dr. Alexandre Dauphin** and **ICREA Prof. Maciej Lewenstein**; M. N. Mikheev Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences; King's College London; University of Salamanca; Max Planck POSTECH/KOREA Research Initiative and Condensed Matter Physics Center (IFIMAC), presented a complementary scheme to ARPES in Reports on Progress in Physics Original Research. In a numerical experiment supported by a theoretical model, the team demonstrated that **X-ray absorption spectroscopy can directly capture topological phase transitions**.

The method employs ultrashort probe pulses that do not suffer from energy resolution reduction. This approach enables further studies of relevant systems for optoelectronics applications, whose investigation had so far been held back by the duration/resolution trade-off.

Topological phase transitions leave an absorption trace

The researchers simulated the action of two ultrashort pulses, separated by a time delay, on a hexagonal boron-nitrate monolayer (hBN). One of them was a linearly-polarized x-ray pulse and the other a circularly-polarized intense infrared pulse. By changing the circular polarization of the latter from left- to right-handed, the absorption of the sample also changed. This dependence enabled them to infer the topological phase of the material.

i¿½Our ultrafast scheme was very sensitive to topological phase transitions. When t e topological phase changed, there was a sign imprinted in the absorption spectrumi?½, explains ICREA Prof. Maciej Lewenstein. i¿½Therefore, this method could be used to study topological phases and identify topological phase transitions within some materials. N w, we need an experimental design to be able to demonstrate it in a real-case scenar

Reference:
Juan F P Mosquera et al 2024 Rep. Prog. Phys. **87** 11790
DOI: 10.1088/1361-6633/ad889

Acknowledgements:
J.F.P.M, G.C., M.M., and A.P. acknowledge Comunidad de Madrid through TALENTO grant refs. 2017-T1/IND-5432 and 2021-5A/IND-20959, and the Spanish Ministry of Science, Innovation and Universities & the State Research Agency through grants refs. PID2021-126560NB-I00 and CNS2022-135803 (MCIU/AEI/FEDER, UE), and the i¿½Maria e Maeztui¿½ Programme for Units of Excellence in R&D (CEX2023-001316-M), and FASL GHT network (RED2022-134391-T), and computer resources and assistance provided by Centr de Computacion Cientifica de la Universidad Autonoma de Madrid (FI-2021-1-0032), Institut de Biocomputacion y Fisica de Sistemas Complejos de la Universidad de Zara oza (FI-2020-3-0008), and Barcelona Supercomputing Center (FI-2020-1-0005, FI2021-2-0 23, FI-2021-3-0019). This publication is based upon work from COST Action NEXT, CA2 148 supported by COST (European Cooperation in Science and Technology). M. Malakhov's ork also carried out within the state assignment of Ministry of Science and Higher Educatio of the Russian Federation (theme i¿½Quantumi¿½ No. 122021000038-7). E.P. ackn wledges Royal Society funding under URF\R1\211390, RF\ERE\210255 and RF\ERE\231081. CFO and ex-ICFO co-authors acknowledge Europea Research Council AdG NOQIA; CIN/AEI (PGC2018-0910.13039/501100011033, CEX2019-000910-S/10.13039/5011000110 3, Plan National FIDEUA PID2019-106901GB-I00, Plan National STAMEENA PID2022-139099 B, I00, project funded by MCIN/AEI/10.13039/501100011033 and by the i¿½Euro ean Union NextGenerationEU/PRTRi¿½ (PRTRC17.I1), FPI); QUANTERA MAQS PCI201 -111828-2); QUANTERA DYNAMITE PCI2022-132919, QuantERA II Programme co-funded by European Union's Horizon 2020 program under Grant Agreement No 101017733); Ministry for Digital Transformation and of Civil Service of the Spanish Government through the UANTUM ENIA project call - Quantum Spain project, and by the European Union through t e Recovery, Transformation and Resilience Plan - NextGenerationEU within the framework of the Digital Spain 2026 Agenda; Fundacio Cellex; Fundacio Mir-Puig; Generalitat de Catalun a (European Social Fund FEDER and CERCA program, AGAUR Grant No. 2021 SGR 01452

QuantumCAT U16-011424, co-funded by ERDF Operational Program of Catalonia 2014-2020
; Barcelona Supercomputing Center MareNostrum (FI-2023-3-0024); Funded by the Eur
pean Union. (HORIZON-CL4-2022-QUANTUM-02-SGA PASQuanS2.1, 101113690, EU
orizon 2020 FETOPEN OPTOlogic, Grant No 899794), EU Horizon Europe Program (This
project has received funding from the European Union's Horizon Europe research an
innovation program under grant agreement No 101080086 NeQSTGrant Agreeme
t 101080086 -NeQST); ICFO Internal i¿½QuantumGaudii¿½ project; European Unio
's Horizon 2020 program under the Marie Sklodowska-Curie grant agreement No 847648
i¿½La Caixai¿½ Junior Leaders fellowships, La Caixai¿½ Foundation (ID 100010434)
CF/BQ/PR23/11980043. A.C. thanks to the Sistema Nacional de Investigacion (SNI) de Panama for financial s