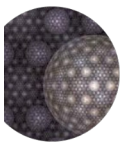


Experimental demonstration of a magnetically induced warping transition in a topological insulator mediated by rare-earth surface dopants

Beatriz Muñiz Cano

Spin-ARPES Laboratory, IMDEA Nanociencia, Madrid, Spain

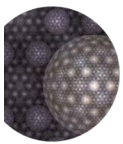
AUSE Meeting 2024



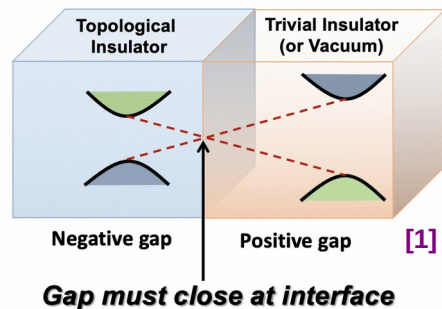
Introduction: topological insulators (TIs)

w w w . n a n o s c i e n c e . i m d e a . o r g

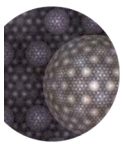




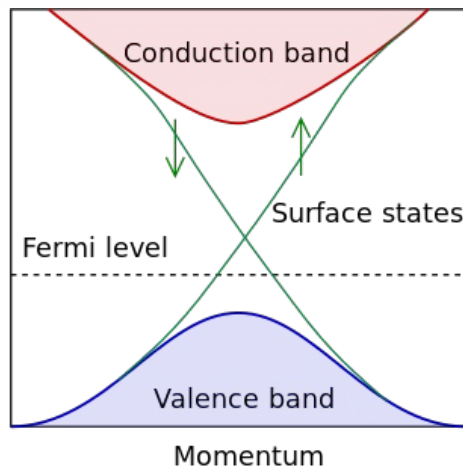
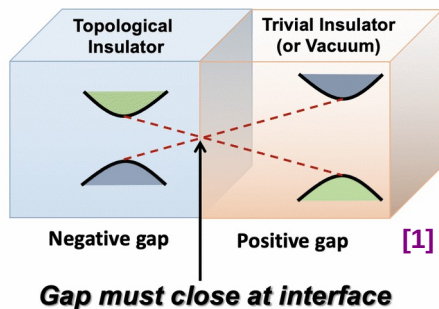
Introduction: topological insulators (TIs)



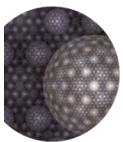
- Topological insulators (TIs) → bulk insulators + **conducting linearly dispersing Dirac edge (surface) states**



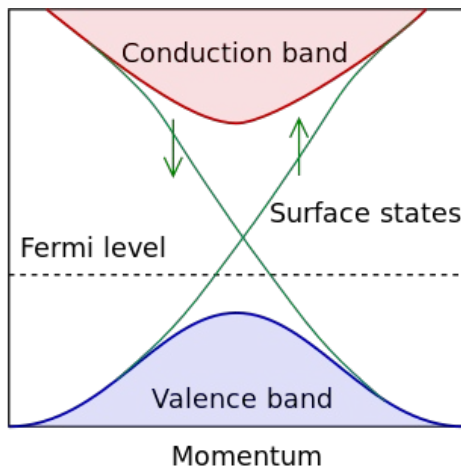
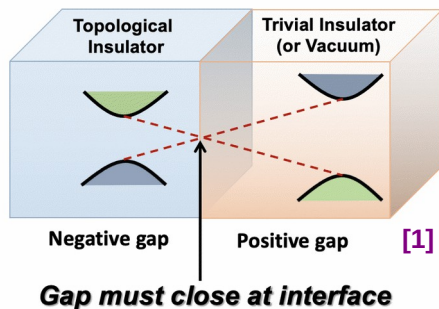
Introduction: topological insulators (TIs)



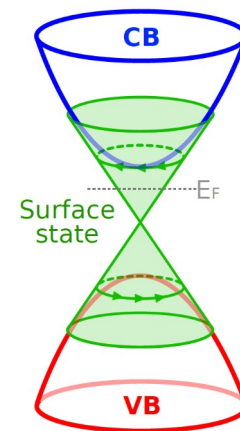
- Topological insulators (TIs) → bulk insulators + conducting linearly dispersing Dirac edge (surface) states
- **Surface states (SS) are topologically protected by time-reversal symmetry (TRS) → topological SS (TSS)**

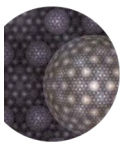


Introduction: topological insulators (TIs)

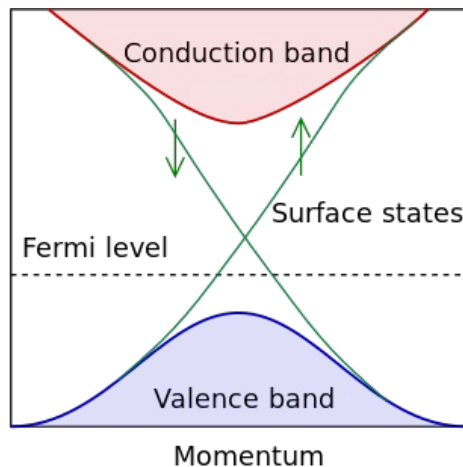
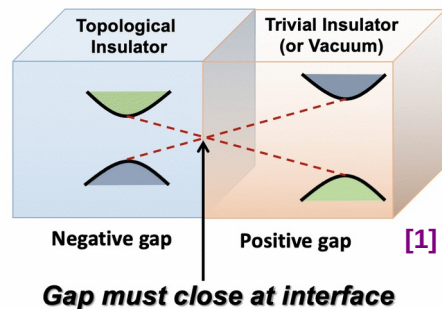


- Topological insulators (TIs) → bulk insulators + conducting linearly dispersing Dirac edge (surface) states
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- **Large spin-orbit coupling (SOC)**

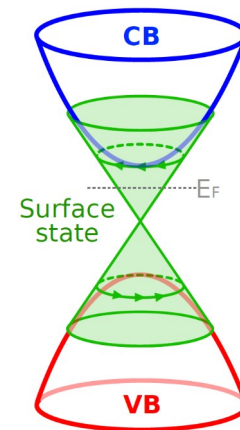


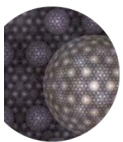


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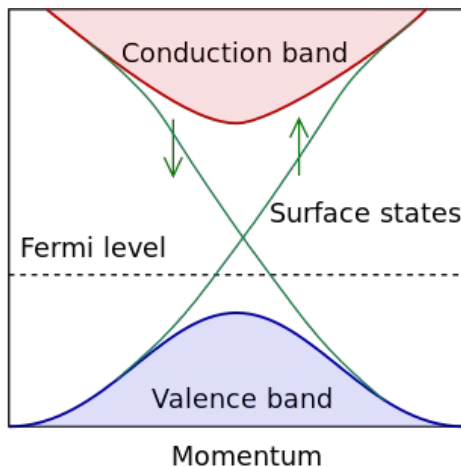
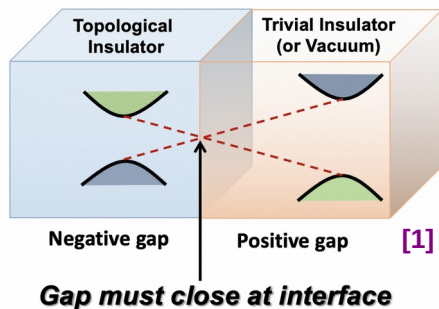


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- **Topologic robustness** + exotic properties → **spintronics, quantum computing**

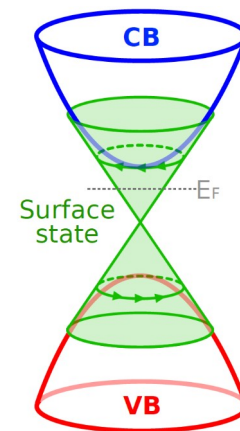




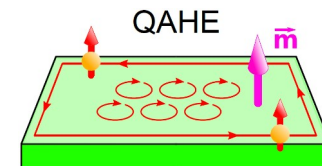
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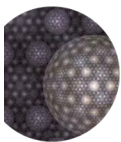


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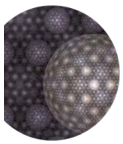
Disipationless spin-polarized currents
(insulating inside y
conductive en el edge)





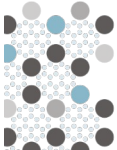
Introduction: magnetic TIs (MTIs)

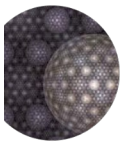




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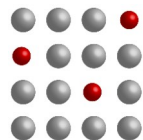
- Impurity magnetic doping



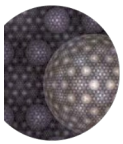


Introduction: magnetic TIs (MTIs)

- Impurity magnetic doping

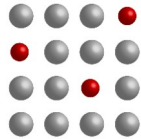


Substitutional or
surface doping [2]

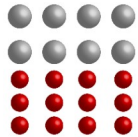


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- Impurity magnetic doping

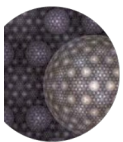


Substitutional or
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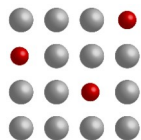
Proximity coupling [3]

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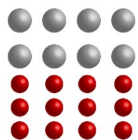


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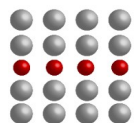
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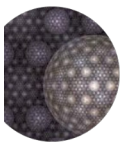
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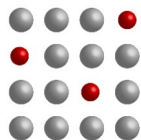


Magnetic extension [4]

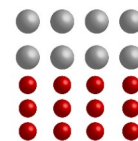


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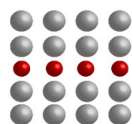
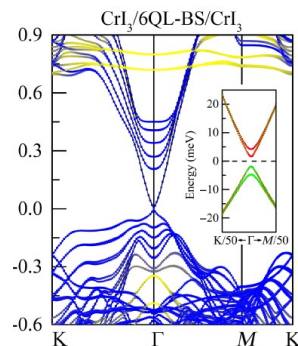
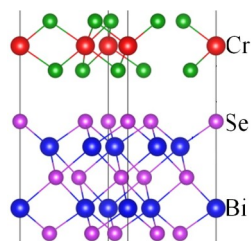
- Impurity magnetic doping



Substitutional or
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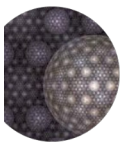


Proximity coupling [3]



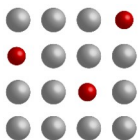
Magnetic extension [4]

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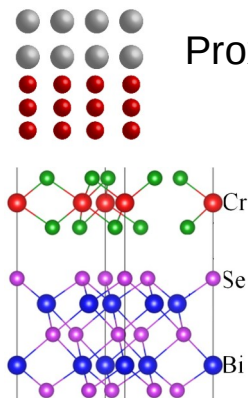


Introduction: magnetic TIs (MTIs)

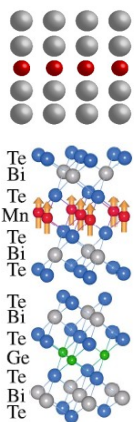
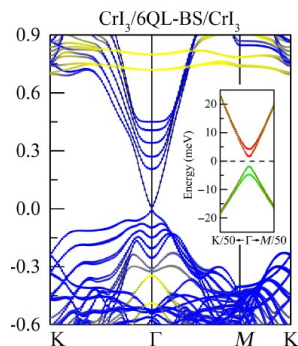
• Impurity magnetic doping



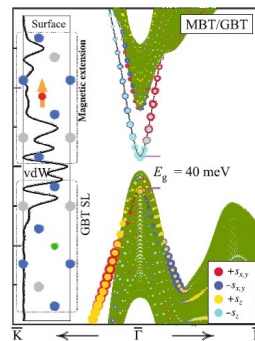
Substitutional or
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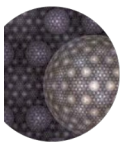
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Magnetic extension [4]

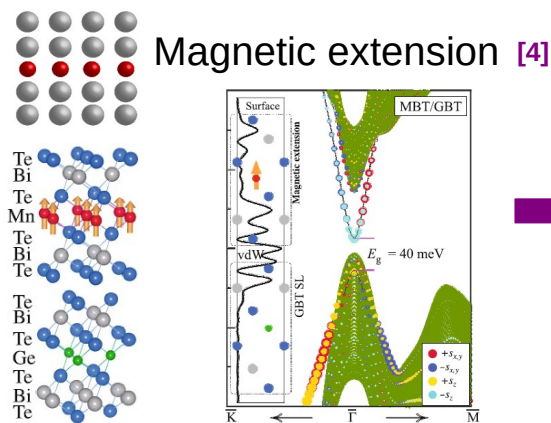
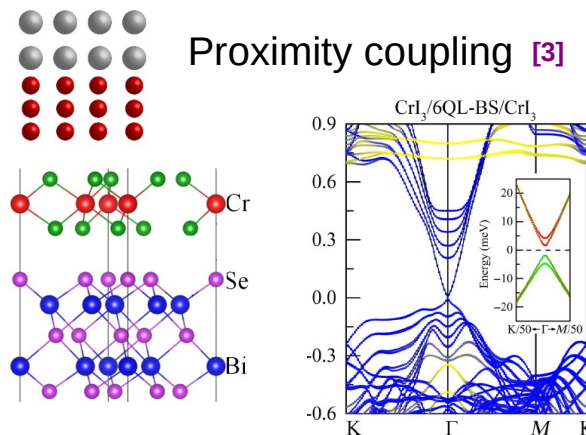
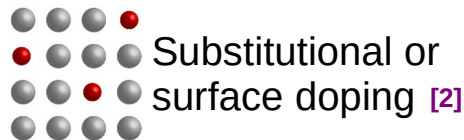


[2] Chen, Y. et al. *Science* **2010**, 329, 659–662. [3] Hou, Y et al. *Science adv.* **2019**, 5, eaaw1874. [4] Otrokov, M. M. et al. *JETP Lett.* **2017**, 105, 297–302.



Introduction: magnetic TIs (MTIs)

• Impurity magnetic doping



Prediction and observation of an antiferromagnetic topological insulator [5]

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Large magnetic gap at the Dirac point in Bi₂Te₃/MnBi₂Te₄ heterostructures [6]

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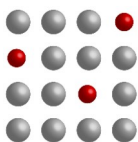
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[2] Chen, Y. et al. Science **2010**, 329, 659–662. [3] Hou, Y et al. Science adv. **2019**, 5, eaaw1874. [4] Otrokov, M. M. et al. JETP Lett. **2017**, 105, 297–302. [5] Otrokov, M. M. et al. Nature **2019**, 576, 416–422. [6] Rienks, E. D. et al. Nature **2019**, 576, 423–428.

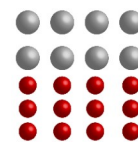


Introduction: magnetic TIs (MTIs)

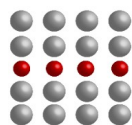
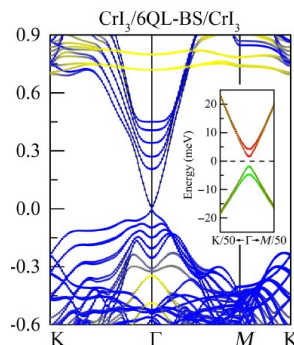
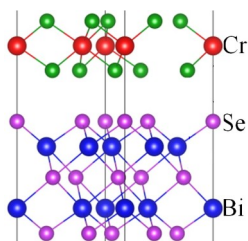
• Impurity magnetic doping



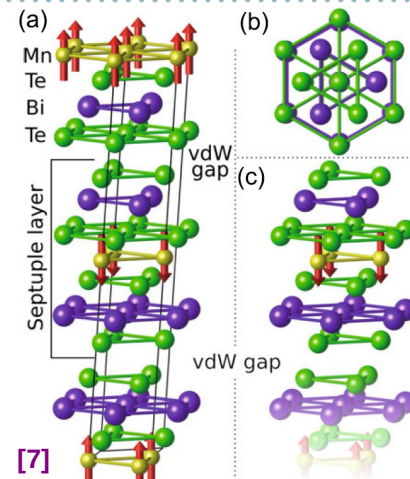
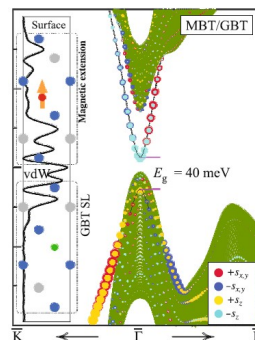
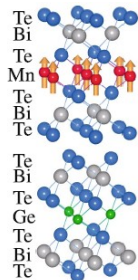
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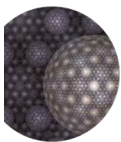
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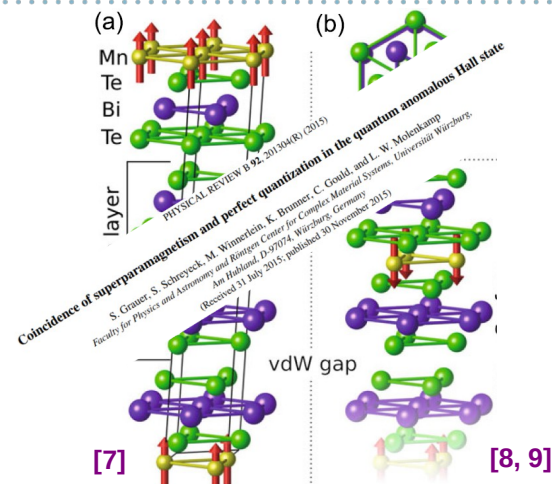
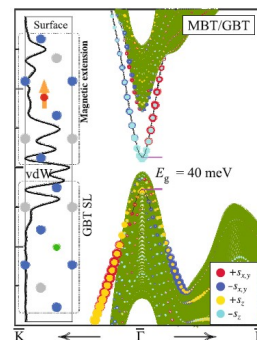
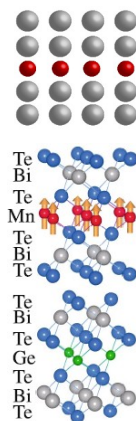
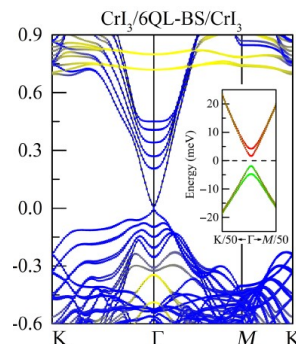
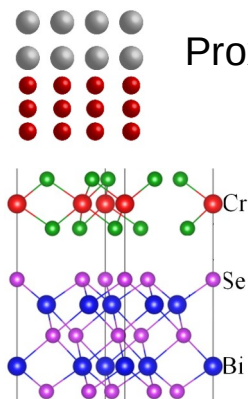
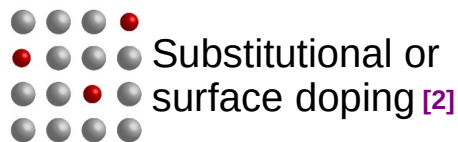


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Introduction: magnetic TIs (MTIs)

• Impurity magnetic doping



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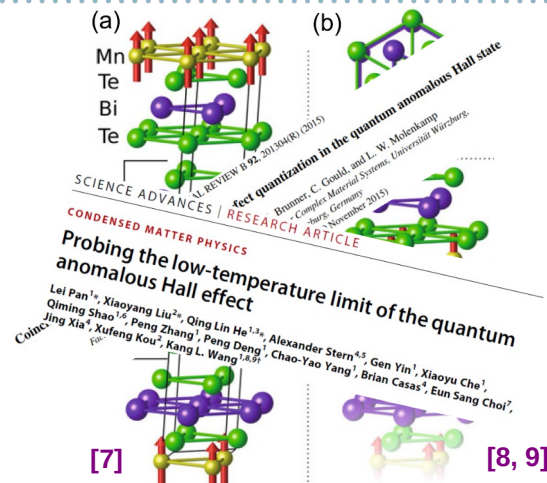
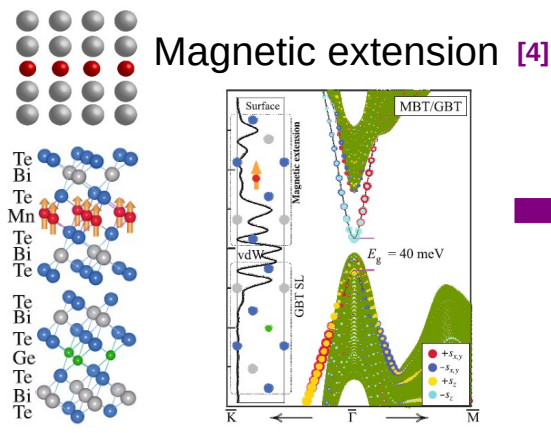
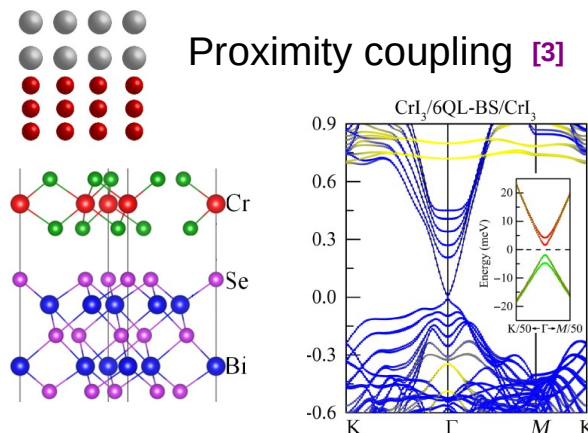
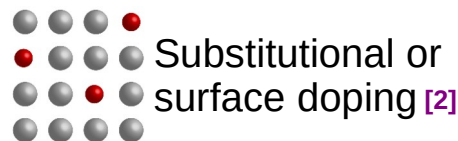
E. D. L. Rienks^{1,2,3,4*}, S. Wimmer^{4,14}, J. Sánchez-Barriga^{4,14}, O. Caha^{4,14}, P. S. Mandal¹⁷, J. Růžická⁴, A. Ney⁴, H. Steiner⁴, V. V. Volobuev^{4,14}, H. Grotis⁴, M. Albu⁴, G. Köhler⁴, J. Michalická⁴, S. A. Khan⁴, J. Minár⁴, H. Ebert⁴, G. Bauer⁴, F. Freyse⁴, A. Varykhalov⁴, O. Rader⁴ & G. Springholz⁴



[2] Chen, Y. et al. Science **2010**, 329, 659–662. [3] Hou, Y et al. Science adv. **2019**, 5, eaaw1874. [4] Otrokov, M. M. et al. JETP Lett. **2017**, 105, 297–302. [5] Otrokov, M. M. et al. Nature **2019**, 576, 416–422. [6] Rienks, E. D. et al. Nature **2019**, 576, 423–428. [7] Garnica, M. et al. Npj Quant. Mat. **2022**, 7, 1–9. [8] Grauer, S. et al. PRB **2015**, 92, 201304. [9] Pan, L. et al. Science adv. **2020**, 6, eaaz3595.

Introduction: magnetic TIs (MTIs)

• Impurity magnetic doping



Prediction and observation of an antiferromagnetic topological insulator [5]

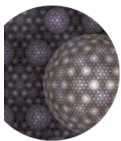
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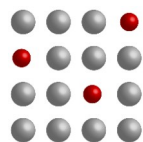


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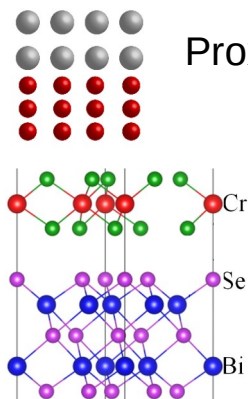


Introduction: magnetic TIs (MTIs)

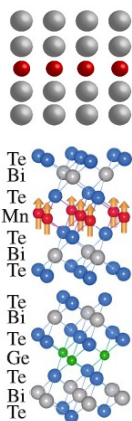
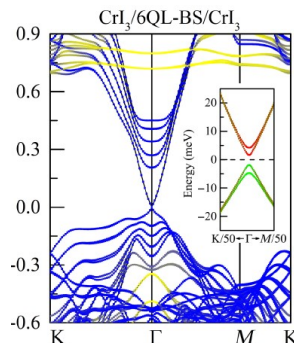
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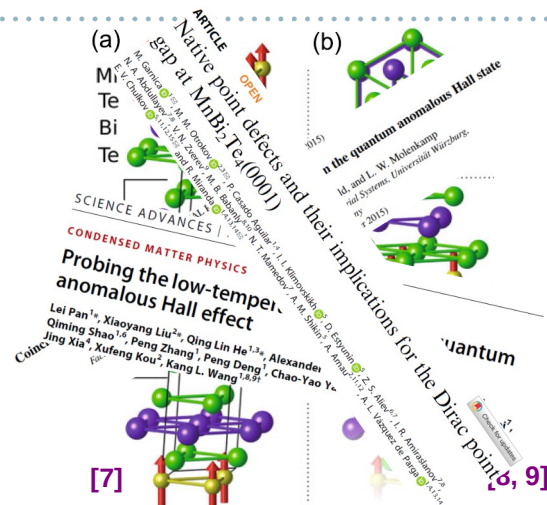
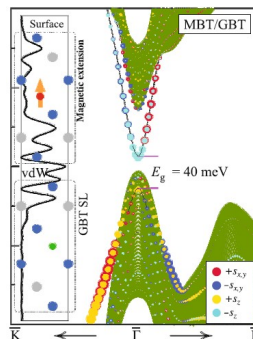
Substitutional or
surface doping [2]



Proximity coupling [3]



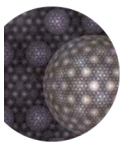
Magnetic extension [4]



Prediction and observation of an
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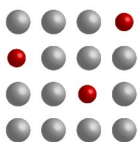
Large magnetic gap at the Dirac point in
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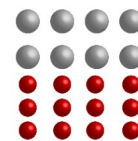
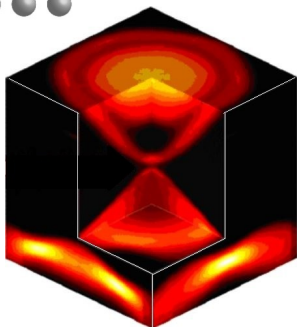


Introduction: magnetic TIs (MTIs)

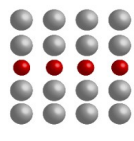
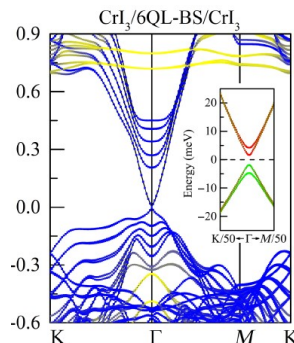
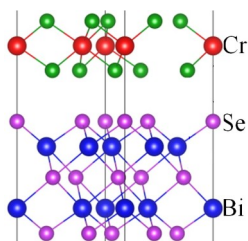
• Impurity magnetic doping



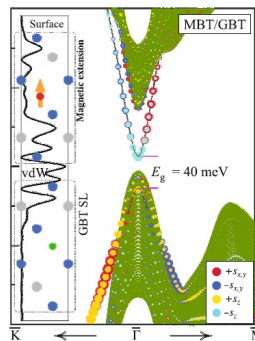
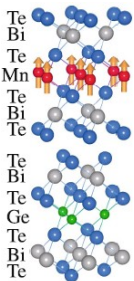
Substitutional or
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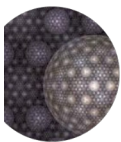
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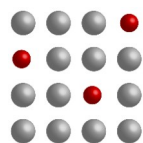
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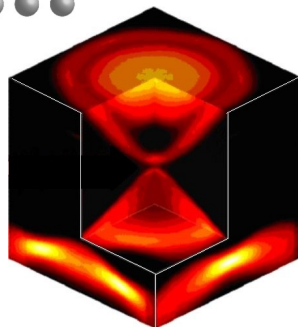


Introduction: magnetic TIs (MTIs)

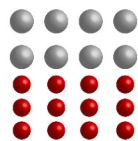
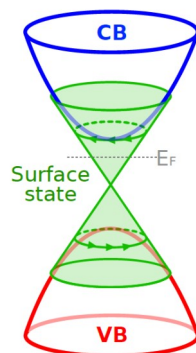
• Impurity magnetic doping



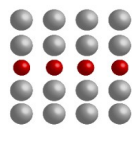
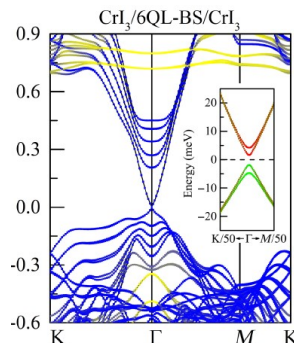
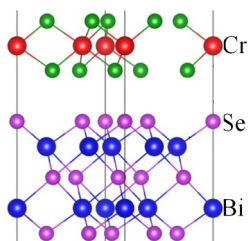
Substitutional or
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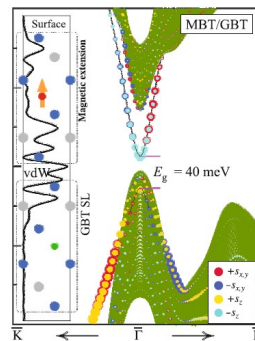
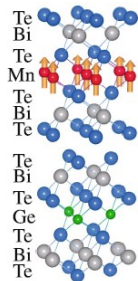
Massless Dirac
fermions



Proximity coupling [3]

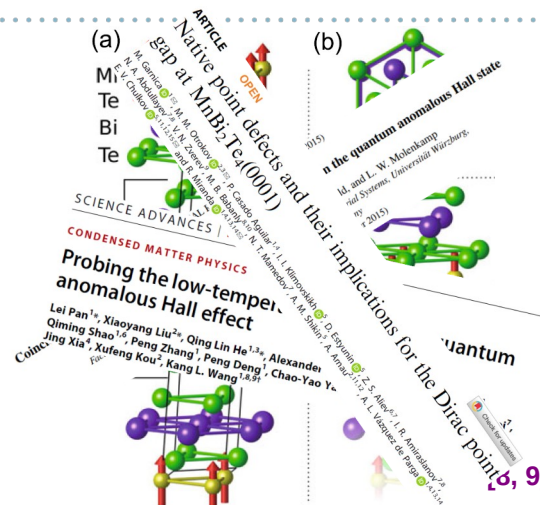


Magnetic extension [4]

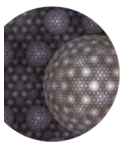


Prediction and observation of an
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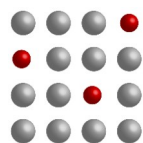


[2] Chen, Y. et al. *Science* **2010**, 329, 659–662. [3] Hou, Y et al. *Science adv.* **2019**, 5, eaaw1874. [4] Otrokov, M. M. et al. *JETP Lett.* **2017**, 105, 297–302. [5] Otrokov, M. M. et al. *Nature* **2019**, 576, 416–422. [6] Rienks, E. D. et al. *Nature* **2019**, 576, 423–428. [7] Garnica, M. et al. *Npj Quant. Mat.* **2022**, 7, 1–9. [8] Grauer, S. et al. *PRB* **2015**, 92, 201304. [9] Pan, L. et al. *Science adv.* **2020**, 6, eaaz3595.

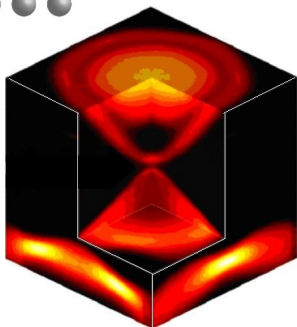


Introduction: magnetic TIs (MTIs)

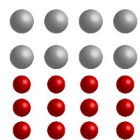
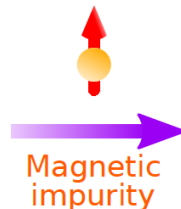
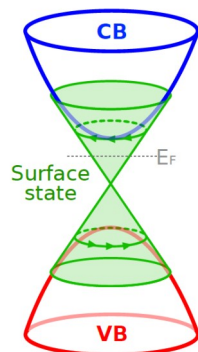
• Impurity magnetic doping



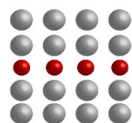
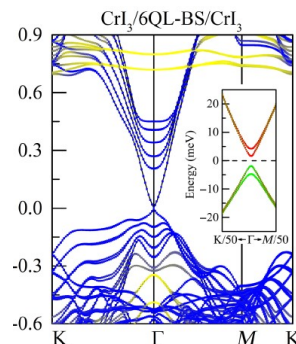
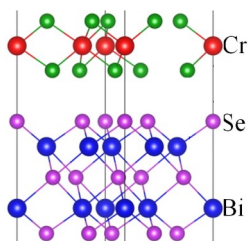
Substitutional or
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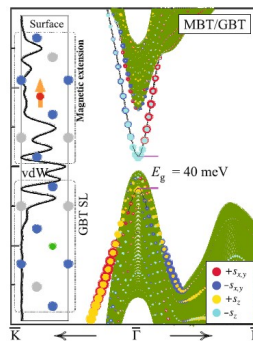
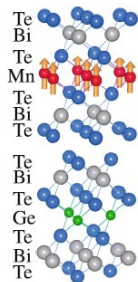
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M. M. Otrokov^{1,2,3,4,*}, I. I. Klimovskikh¹, H. Bentmann⁵, D. Estyunin¹, A. Zengner¹, Z. S. Aliev^{1,2}, S. Gao⁵, A. Li⁶, B. Wolter⁵, A. V. Koroleva¹, A. M. Shik¹, M. Blanco-Ruiz^{1,2}, M. Hoffmann¹, I. P. Rusinov^{1,2}, A. Yu. Vyazovskaya^{4,12}, S. V. Eremin^{1,2,13}, Yu. M. Koroteev^{1,2,13}, V. M. Kuznetsov¹, F. Freyse¹⁴, J. Sánchez-Barriga¹⁴, R. A. Amiraslanov¹, M. B. Babani¹⁵, N. T. Mamedov¹⁶, N. A. Abdullayev¹, V. N. Zverev¹, A. Alfonso¹, V. Kataev¹, M. Koroteev^{1,2,13}, E. F. Schiav¹⁸, S. Kumar¹⁹, A. Kimura²⁰, L. Petaccia²¹, G. Di Santo²², R. C. Vidal²³, S. Schatzl²⁴, K. Kilner²⁵, M. Unzelm²⁶, C. H. Min²⁷, Simon Moser²⁸, T. R. F. Peixoto²⁹, F. Reinert³⁰, A. Ernst^{31,32}, P. M. Echenique^{33,34}, A. Isaeva³⁵ & E. V. Chulkov^{34,36}

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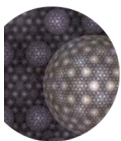
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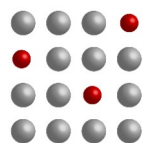


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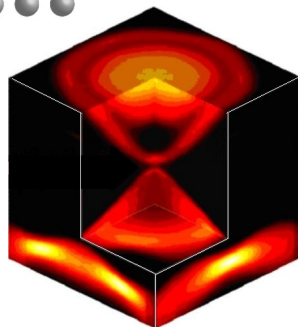


Introduction: magnetic TIs (MTIs)

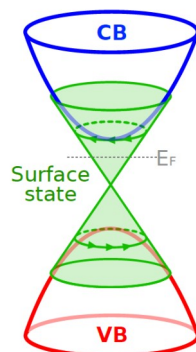
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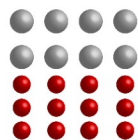
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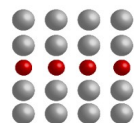
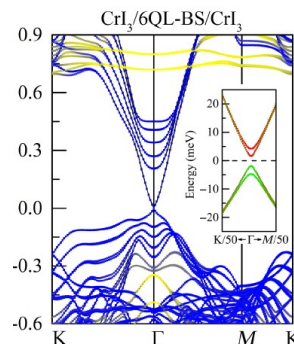
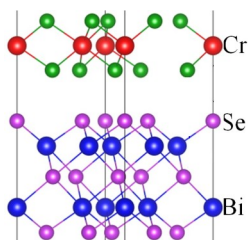
TRS
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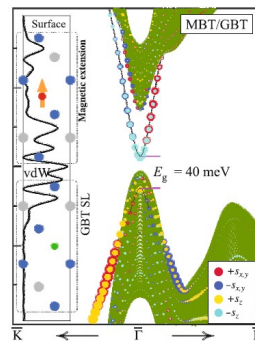
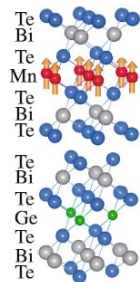
Magnetic
impurity



Proximity coupling [3]

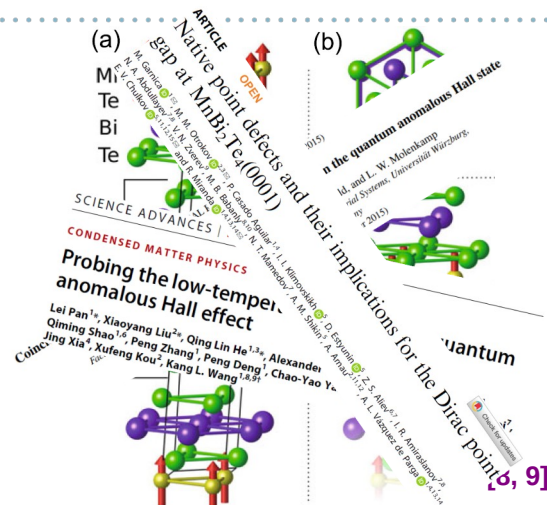


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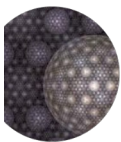


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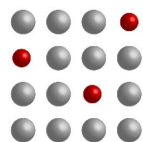


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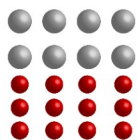
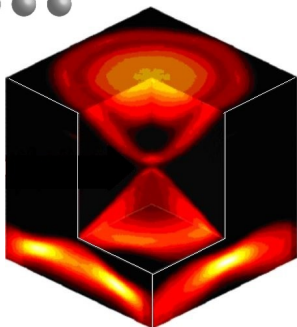


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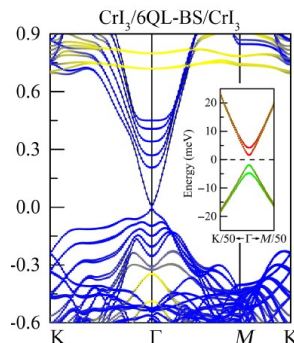
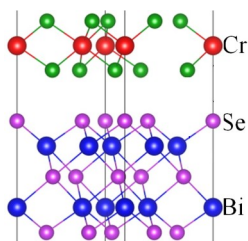
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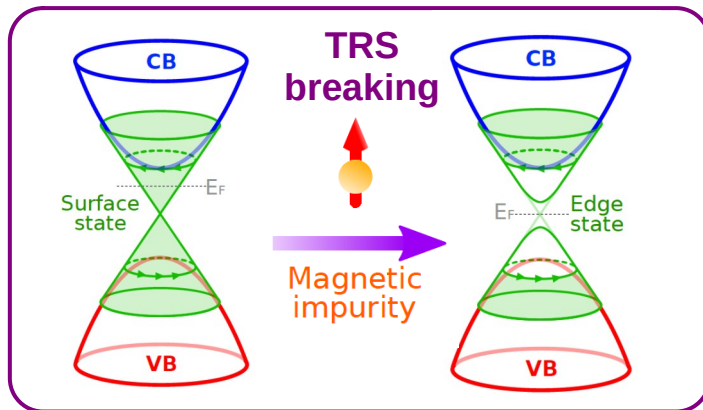
Substitutional or
surface doping [2]



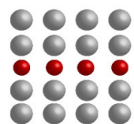
Proximity coupling [3]



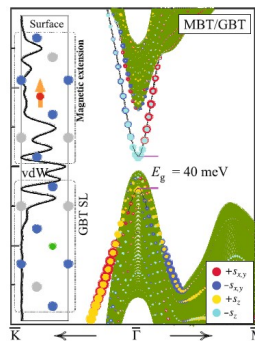
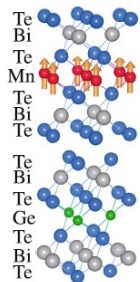
Massless Dirac
fermions



Massive Dirac
fermions



Magnetic extension [4]



Prediction and observation of an
antiferromagnetic topological insulator [5]

<https://doi.org/10.1038/s41566-019-1840-9>
M. M. Otrokov^{1,2,3,4,*}, I. I. Klimovskikh¹, H. Bentmann⁵, D. Estyunin¹, A. Zengner¹, Z. S. Aliev^{1,8}, S. Gao¹, A. Li¹, B. Wolter¹, A. V. Koroleva¹, A. M. Shik¹, M. Blanco-Ruiz^{1,9}, M. Hoffmann¹, I. P. Rusinov^{1,10}, A. Yu. Vyazovskaya^{4,10}, S. V. Eremin^{1,11,12}, Yu. M. Koroteev^{1,12}, V. M. Kuznetsov¹, F. Freyse¹⁴, J. Sánchez-Barriga¹⁴, I. R. Amiraslanov¹, M. B. Babani¹⁵, N. T. Mamedov¹⁶, N. A. Abdullayev¹⁷, V. N. Zverev¹⁸, A. Alfonso¹⁹, V. Kataev¹⁹, B. Büchner²⁰, E. F. Schiav²¹, S. Kumar²², A. Kimura²³, L. Petaccia²⁴, G. Di Santo²⁵, R. C. Vidal²⁶, S. Schatz²⁷, K. Kilner²⁸, M. Unalimani²⁹, C. H. Min³⁰, Simon Moser³¹, T. R. P. Peixoto³², F. Reinert³³, A. Ernst^{34,35}, P. M. Echenique^{1,36}, A. Isaeva³⁷ & E. V. Chulkov^{1,40,41}

Received: 20 September 2018
Accepted: 18 September 2019
Published online: 18 December 2019

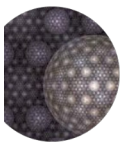
Large magnetic gap at the Dirac point in
Bi₂Te₃/MnBi₂Te₄ heterostructures [6]

<https://doi.org/10.1038/s41566-019-1826-7>
E. D. Rienks^{1,2,3,4,*}, S. Wimmer^{4,5,6}, J. Sánchez-Barriga^{1,4}, O. Caba^{5,6}, P. S. Mandal^{1,7}, J. Růžicka⁸, A. Ney⁸, H. Steinle⁹, V. V. Volobuev^{4,10,11}, H. Groiss⁸, M. Albu¹⁰, G. Kothleitner¹⁰, J. Michalicka¹⁰, S. A. Khan¹¹, J. Minář¹¹, H. Ebert¹², G. Bauer¹³, F. Freyse¹⁴, A. Varykhalov¹⁵, O. Rader¹⁶ & G. Springholz¹⁴

Received: 10 May 2018
Accepted: 18 October 2019
Published online: 18 December 2019

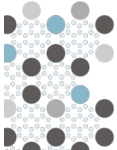


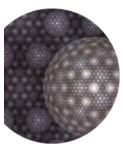
[2] Chen, Y. et al. *Science* **2010**, 329, 659–662. [3] Hou, Y et al. *Science adv.* **2019**, 5, eaaw1874. [4] Otrokov, M. M. et al. *JETP Lett.* **2017**, 105, 297–302. [5] Otrokov, M. M. et al. *Nature* **2019**, 576, 416–422. [6] Rienks, E. D. et al. *Nature* **2019**, 576, 423–428. [7] Garnica, M. et al. *Npj Quant. Mat.* **2022**, 7, 1–9. [8] Grauer, S. et al. *PRB* **2015**, 92, 201304. [9] Pan, L. et al. *Science adv.* **2020**, 6, eaaz3595.



Introduction: surface magnetic doping: 3d magnetic impurities

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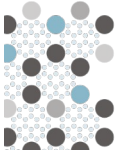
Introduction: surface magnetic doping: 3d magnetic impurities

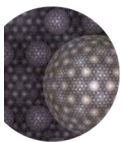
www.nanoscience.imdea.org



Growth

Doping

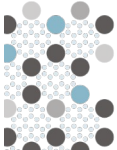


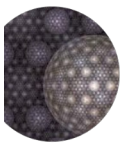


Introduction: surface magnetic doping: 3d magnetic impurities

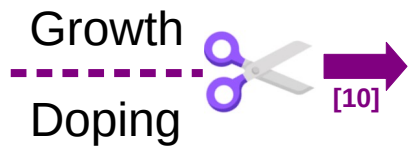
Growth

Doping

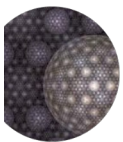




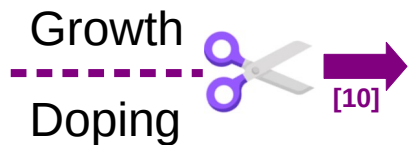
Introduction: surface magnetic doping: 3d magnetic impurities



Limiting dopants to TSSs most sensitive regions
Maximizing magnetic anisotropy by the lower coordination symmetry



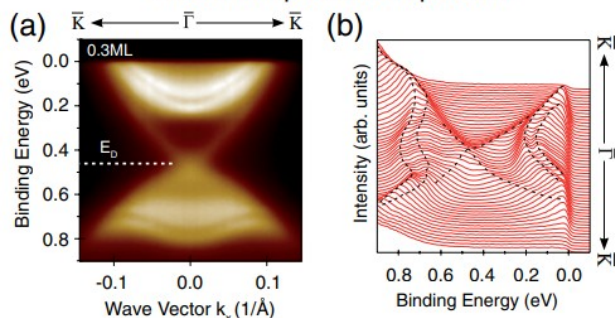
Introduction: surface magnetic doping: 3d magnetic impurities



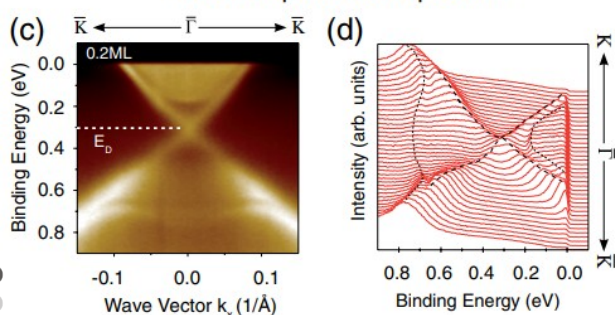
Limiting dopants to TSSs most sensitive regions
Maximizing magnetic anisotropy by the lower coordination symmetry

Multiple adsorption sites [11]

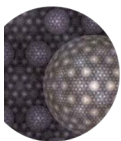
Room-Temperature Deposition



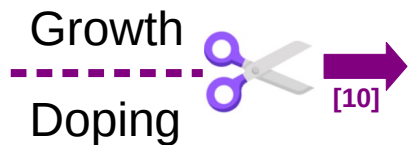
Low-Temperature Deposition



[10] Gambardella, P. et al. Science, **2003**, 300(5622), 1130-1133. [11] Scholz, M. R. et al. Physical Review Letters, **2012**, 108(25), 256810.



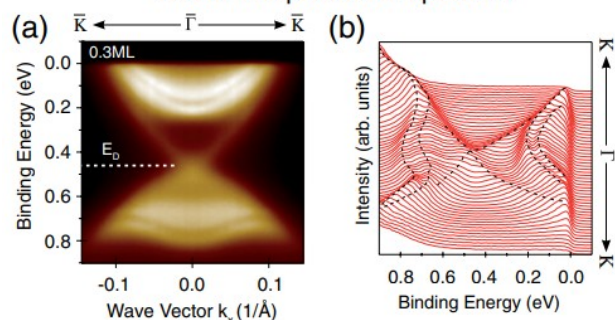
Introduction: surface magnetic doping: 3d magnetic impurities



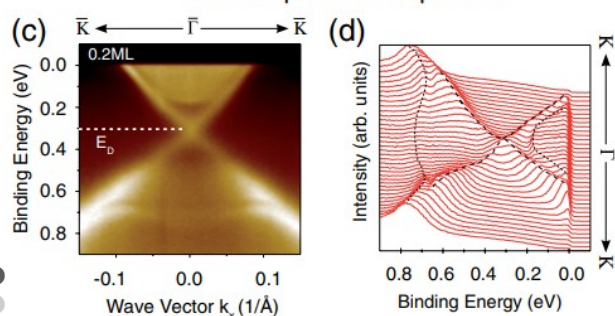
Limiting dopants to TSSs most sensitive regions
Maximizing magnetic anisotropy by the lower coordination symmetry

Multiple adsorption sites [11]

Room-Temperature Deposition



Low-Temperature Deposition



Strong surface relaxations [12]

PHYSICAL REVIEW LETTERS

In-Plane Magnetic Anisotropy of Fe Atoms on Bi₂Se₃(111)

J. Honolka,^{1,*} A. A. Khajetoorians,^{2,†} V. Sessi,³ T. O. Wehling,^{4,5,6} S. Stepanow,¹ J.-L. Mi,⁷ B. B. Iversen,⁷ T. Schlenk,² J. Wiebe,² N. B. Brookes,² A. I. Lichtenstein,⁴ Ph. Hofmann,⁸ K. Kern,^{1,9} and R. Wiesendanger²

¹Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany

²Institute for Applied Physics, Universität Hamburg, D-20355 Hamburg, Germany

³European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble, France

⁴I. Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany

⁵Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, D-28359 Bremen, Germany

⁶Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1a, D-28359 Bremen, Germany

⁷Center for Materials Crystallography, Department of Chemistry, Interdisciplinary Nanoscience Center,

Aarhus University, 8000 Aarhus C, Denmark

⁸Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark

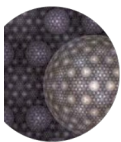
⁹Institut de Physique de la Matière Condensée, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

(Received 20 December 2011; published 22 June 2012)

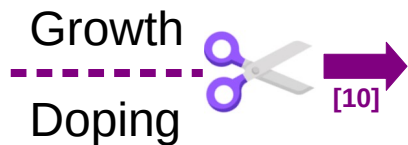
The robustness of the gapless topological surface state hosted by a 3D topological insulator against perturbations of magnetic origin has been the focus of recent investigations. We present a comprehensive study of the magnetic properties of Fe impurities on the prototypical 3D topological insulator Bi₂Se₃ using local low-temperature scanning tunneling spectroscopy and integral x-ray magnetic circular dichroism techniques. Single Fe adatoms on the Bi₂Se₃ surface, in the coverage range $\approx 1\%$ of a monolayer, are heavily relaxed into the surface and exhibit a magnetic easy axis within the surface plane, contrary to what was assumed in recent investigations on the supposed opening of a gap. Using *ab initio* approaches, we demonstrate that an in-plane easy axis arises from the combination of the crystal field and dynamic hybridization effects.

DOI: 10.1103/PhysRevLett.108.256811

PACS numbers: 73.20.At, 68.37.Ef, 71.15.Mb, 78.70.Dm

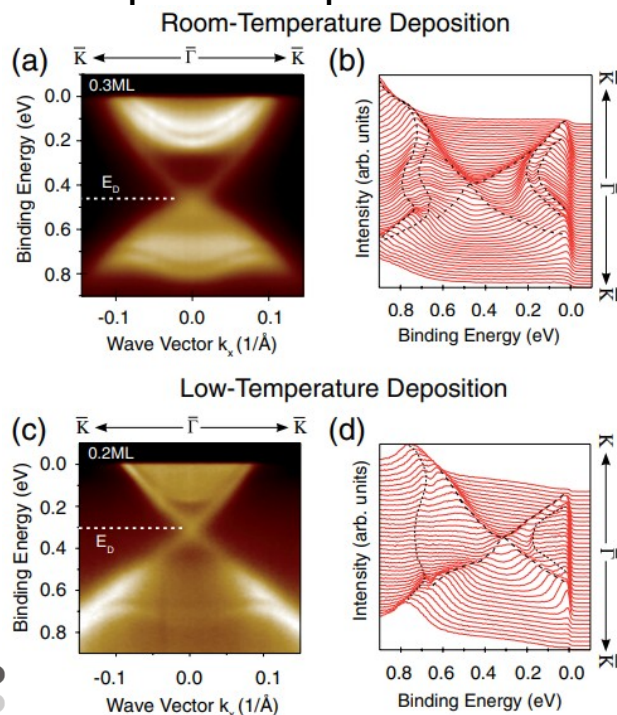


Introduction: surface magnetic doping: 3d magnetic impurities

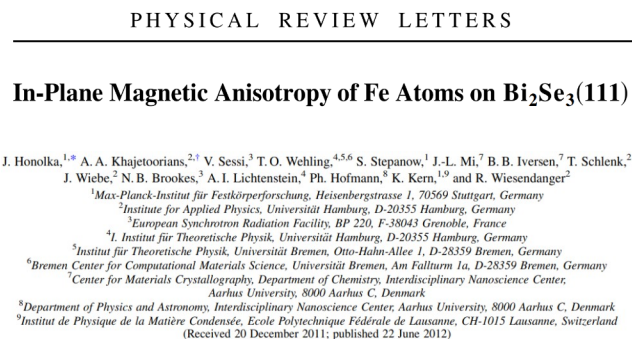


Limiting dopants to TSSs most sensitive regions
Maximizing magnetic anisotropy by the lower coordination symmetry

Multiple adsorption sites [11]



Strong surface relaxations [12]

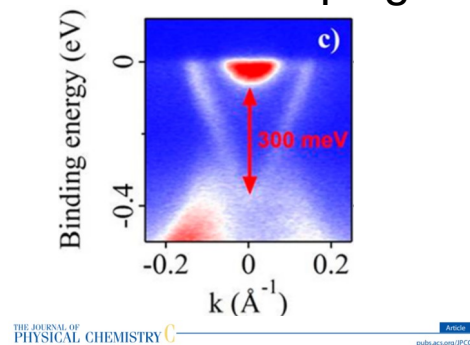


The robustness of the gapless topological surface state hosted by a 3D topological insulator against perturbations of magnetic origin has been the focus of recent investigations. We present a comprehensive study of the magnetic properties of Fe impurities on the prototypical 3D topological insulator Bi_2Se_3 using local low-temperature scanning tunneling spectroscopy and integral x-ray magnetic circular dichroism techniques. Single Fe adatoms on the Bi_2Se_3 surface, in the coverage range $\approx 1\%$ of a monolayer, are heavily relaxed into the surface and exhibit a magnetic easy axis within the surface plane, contrary to what was assumed in recent investigations on the supposed opening of a gap. Using *ab initio* approaches, we demonstrate that an in-plane easy axis arises from the combination of the crystal field and dynamic hybridization effects.

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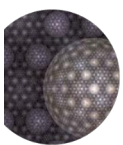
Bulk states doping [13]



Observation of Distinct Bulk and Surface Chemical Environments in a Topological Insulator under Magnetic Doping

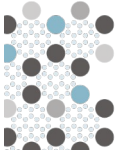
Ivana Vobornik,^{*,1,2} Giancarlo Panaccione,^{*,3,4} Jun Fujii,¹ Zhi-Hai Zhu,³ Francesco Offi,⁵ Benjamin R. Sallés,^{1,2,6} Francesco Borgatti,³ Piero Torelli,³ Jean Pascal Rueff,¹ Denis Cecolin,⁴ Alberto Artioli,¹ Manju Unnikrishnan,³ Giorgio Levy,^{1,2} Massimiliano Marangolo,³ Mamhoud Eddrief,³ Damjan Krizmanic,¹ Huiwen Ji,³ Andrea Damascelli,^{3,7} Gerrit van der Laan,⁸ Russell G. Egglell,⁹ and Robert J. Cava¹

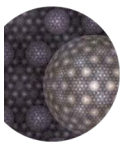
¹Istituto Officina dei Materiali (IOM)-CNR, Laboratorio TASC, Area Science Park, S.S.14, Km 163.5, I-34149 Trieste, Italy
²Department of Physics & Astronomy, University of British Columbia, Vancouver, British Columbia V6T 1Z1, Canada
³Dipartimento di Scienze, Università di Roma Tre, I-00146 Rome, Italy
⁴SMN-CNR, via Gobetti 101, I-40129 Bologna, Italy
⁵Synchrotron SOLEIL, L'Orme des Merisiers, BP 48 Saint-Aubin, 91192 Gif sur Yvette, France
⁶Laboratoire de Chimie Physique – Matière et Rayonnement, Université Pierre et Marie Curie, CNRS, 11 rue Pierre et Marie Curie, 75005 Paris, France
⁷Ministère des NanoSciences de Paris, UPMC–CNRS UMR 7588, 4 place Jussieu, 75252 Paris Cedex 5, France
⁸Department of Chemistry, Princeton University, Princeton, New Jersey 08544, United States
⁹Quantum Matter Institute, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada
¹⁰Diamond Light Source, Chilton, Didcot, Oxfordshire OX11 0DE, United Kingdom
¹¹Department of Chemistry, Inorganic Chemistry Laboratory, University of Oxford, South Parks Road, Oxford OX1 3QR, United Kingdom
¹²International Centre for Theoretical Physics, Strada Costiera 11, 34100 Trieste, Italy



Introduction: rare-earth (RE) surface magnetic doping

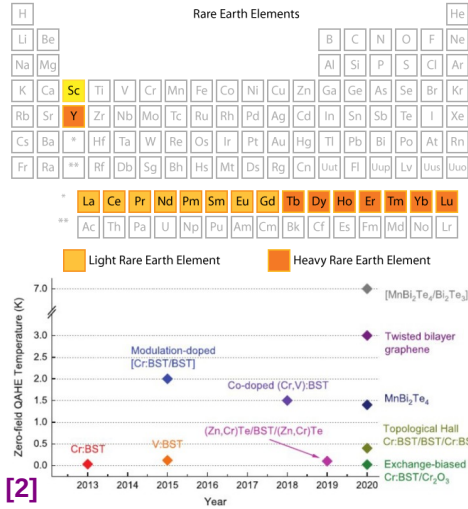
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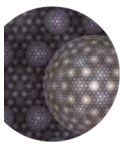




Introduction: rare-earth (RE) surface magnetic doping

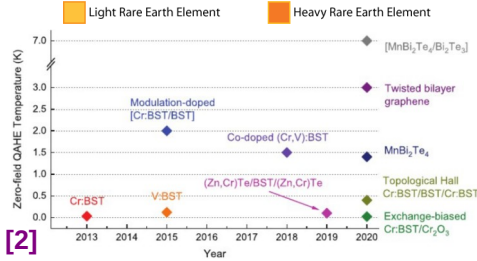
- **Larger size** → prevents from substitutional sites → reduced the multiplicity of adsorption configurations [14]





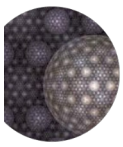
Introduction: rare-earth (RE) surface magnetic doping

H		Rare Earth Elements																He					
Li	Be																	B	C	N	O	F	Ne
Na	Mg																	Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr						
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe						
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn						
Fr	Ra	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo						
		* La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu																					
		** Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr																					



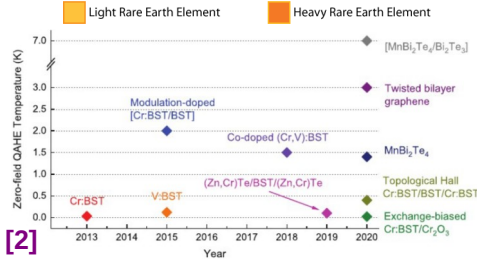
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- Unpaired 4f electrons → **large magnetic moments** → enhanced magnetic anisotropy [15] and allow a lower doping concentration [16]

[14] L. B. Abdalla, et al. PRB, **2013**, 88, 045312. [15] Jensen, J., & Mackintosh, A. R. (1991). Rare earth magnetism (p. 312). Oxford: Clarendon Press. [16] Harrison, S. E. et al. JoP: Cond. Matt., **2015**, 27(24), 245602.



Introduction: rare-earth (RE) surface magnetic doping

Rare Earth Elements																		He					
H																	B	C	N	O	F	Ne	
Li	Be																	Al	Si	P	S	Cl	Ar
Na	Mg																						
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr						
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe						
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn						
Fr	Ra	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo						
* La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu																							
** Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr																							



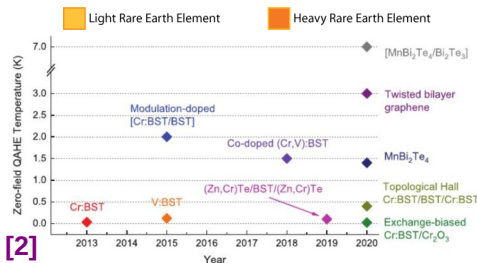
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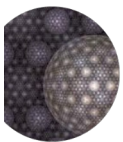
Introduction: rare-earth (RE) surface magnetic doping

Rare Earth Elements

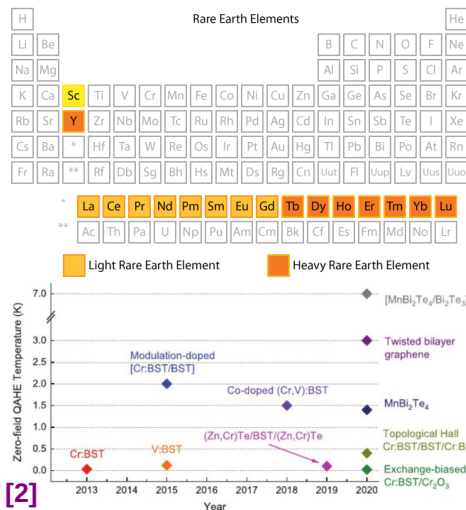
H																	He						
Li	Be																	B	C	N	O	F	Ne
Na	Mg																	Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr						
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe						
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn						
Fr	Ra	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo						
		* LaCePrNdPmSmEuGdTbDyHoErTmYbLu																					
		** AcThPaUNpPuAmCmBkCfEsFmMdNoLr																					



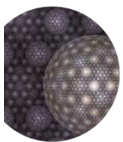
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- **RE substitutional bulk doping:** Eu [18], Gd [19], Ho [20] and Dy [21] on Bi_2Te_3 .



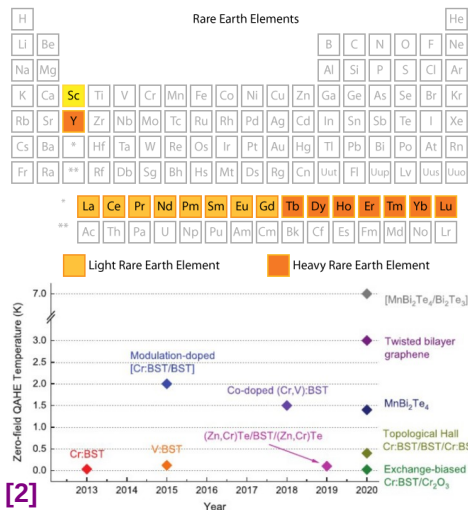
Introduction: rare-earth (RE) surface magnetic doping



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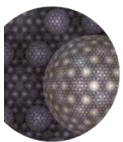


Introduction: rare-earth (RE) surface magnetic doping



Magnetic order in MTIs

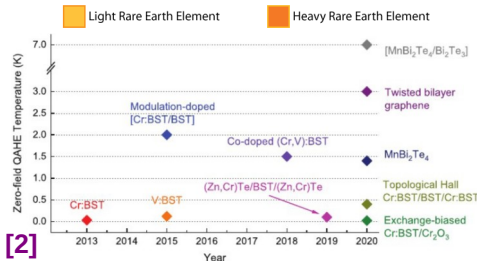
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Introduction: rare-earth (RE) surface magnetic doping

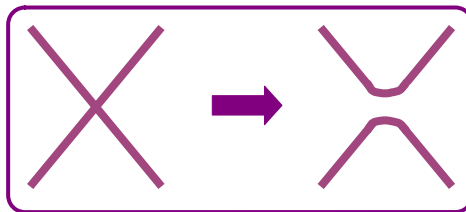
Rare Earth Elements																		He
H																	He	
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K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
Fr	Ra	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo	
		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		

* Light Rare Earth Element ** Heavy Rare Earth Element

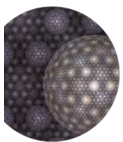


Magnetic
order in MTIs

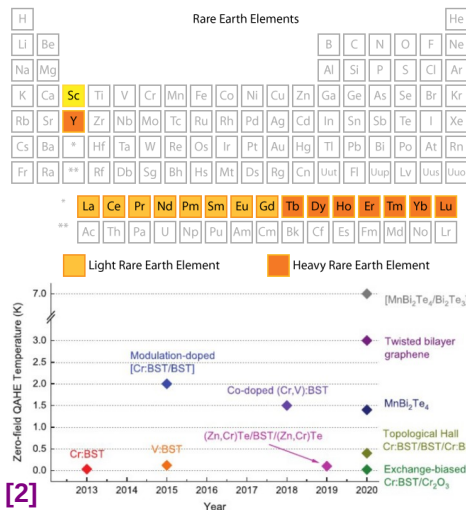
[23, 24]



- Larger size → prevents from substitutional sites → reduced the multiplicity of adsorption configurations [14]
- Unpaired 4f electrons → large magnetic moments → enhanced magnetic anisotropy [15] and allow a lower doping concentration [16]
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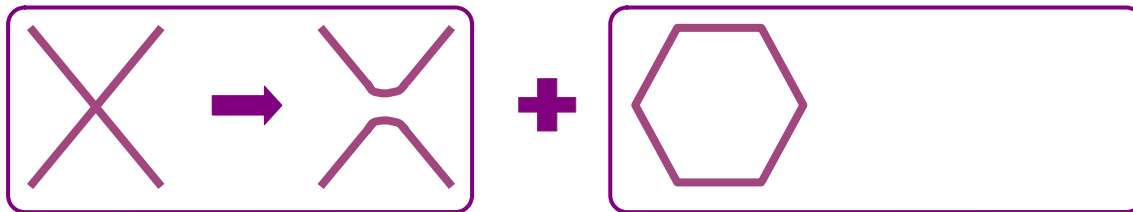


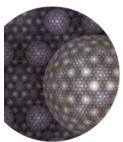
Introduction: rare-earth (RE) surface magnetic doping



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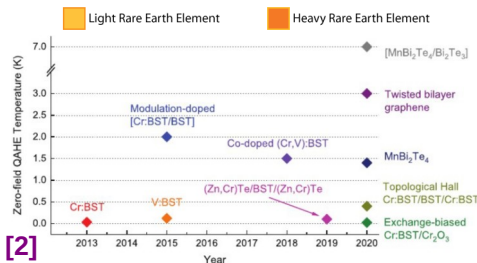
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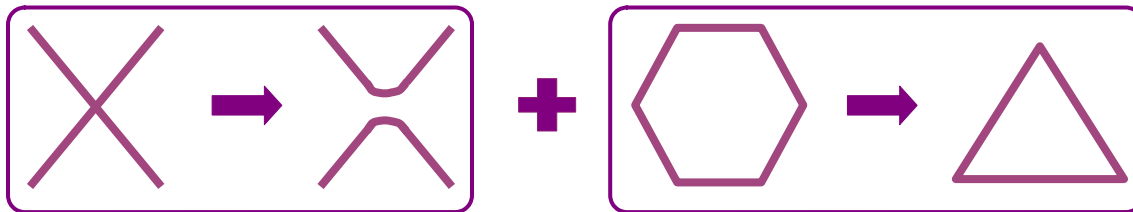
Introduction: rare-earth (RE) surface magnetic doping

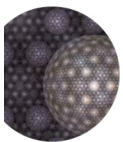
Rare Earth Elements																		He																															
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Li	Be															B	C	N	O	F	Ne																												
Na	Mg															Al	Si	P	S	Cl	Ar																												
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Fr	Ra	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo																																
		<table><tr><td>La</td><td>Ce</td><td>Pr</td><td>Nd</td><td>Pm</td><td>Sm</td><td>Eu</td><td>Gd</td><td>Tb</td><td>Dy</td><td>Ho</td><td>Er</td><td>Tm</td><td>Yb</td><td>Lu</td></tr><tr><td>Ac</td><td>Th</td><td>Pa</td><td>U</td><td>Np</td><td>Pu</td><td>Am</td><td>Cm</td><td>Bk</td><td>Cf</td><td>Es</td><td>Fm</td><td>Md</td><td>No</td><td>Lr</td></tr></table>																La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		
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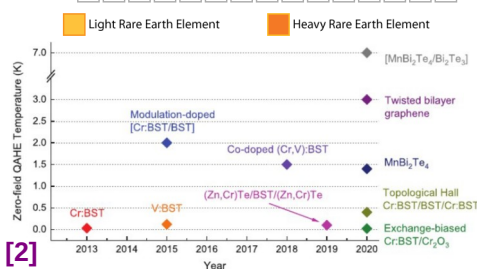
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Rare Earth Elements

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Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo
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*

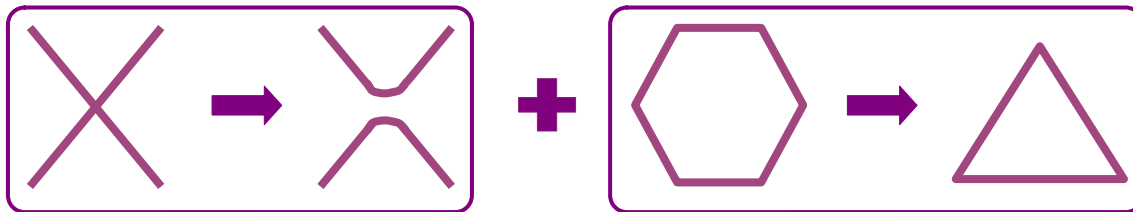
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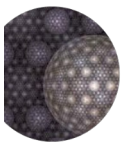
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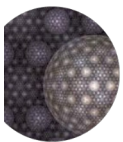
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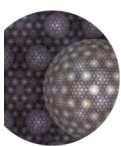


We experimentally report for the first time and theoretically demonstrate such effects on Er-doped $\text{Bi}_2\text{Se}_2\text{Te}$ (BST), along with the tunability of the E_F as a function of the RE coverage, fulfilling the two prerequisites for the realization of the QAHE

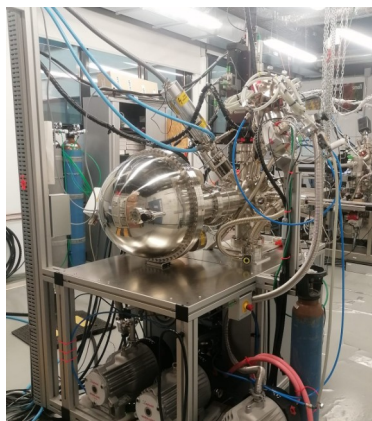
[14] L. B. Abdalla, et al. PRB, **2013**, 88, 045312. [15] Jensen, J., & Mackintosh, A. R. (1991). Rare earth magnetism (p. 312). Oxford: Clarendon Press. [16] Harrison, S. E. et al. J. Phys.: Cond. Matter., **2015**, 27(24), 245602. [17] Omarza M. et al. Nano Lett. **2016**, 16, 7, 4230–4235. [18] Celso I. Fornari et al. J. Phys. Chem. C **2020**, 124, 29, 16048–16057. [19] Kim, J. et al. Sci Rep 5, 2015, 10309. [20] Hesjedal T. et al. physica status solidi (a), **2019**, 216(8), 1800726. [21] S. Harrison et al. J. Phys.: Condens. Matter, **2015**, 27 245602. [22] S. Harrison et al. Sci Rep 5, **2015**, 15767. [23] H. Tanet et al. Phys. Rev. Materials 6, **2022**, 104204. [24] G. Naselli et al. Phys. Rev. Research 4, **2022**, 033198

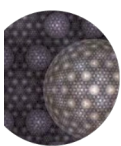




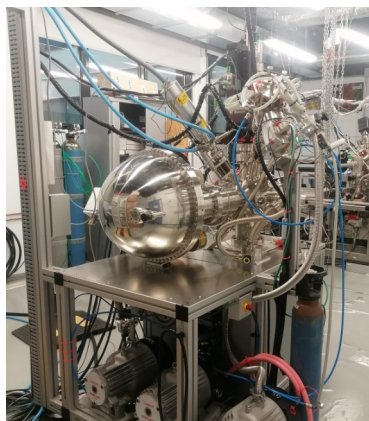


Experimental methods

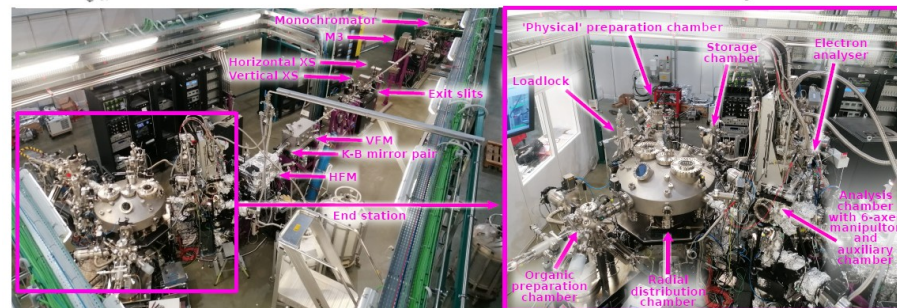
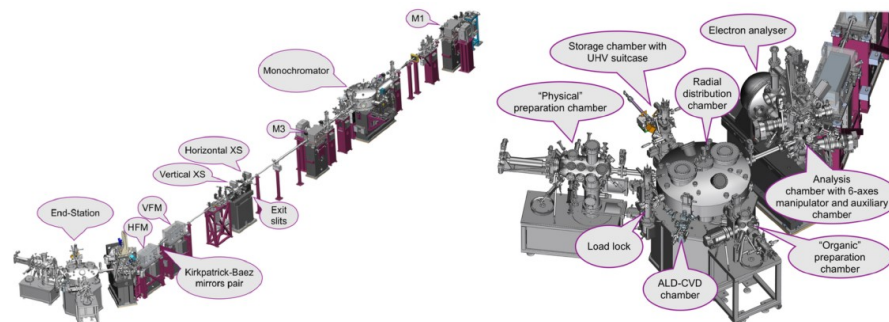




Experimental methods



LOREA beamline

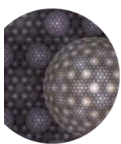


Analysers:

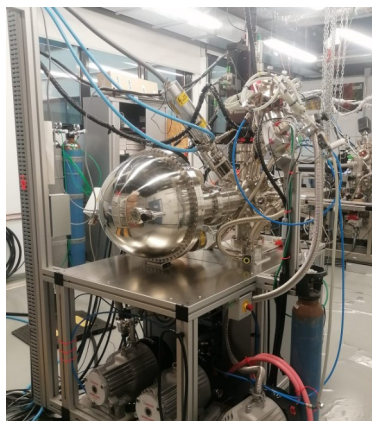
- MBS A-1 hemispherical analyser.
- Resolution better than -1 meV and 0.1° .
- Fast Fermi Surface mapping mode.
- Recently added spin detector.

Cryo-manipulator:

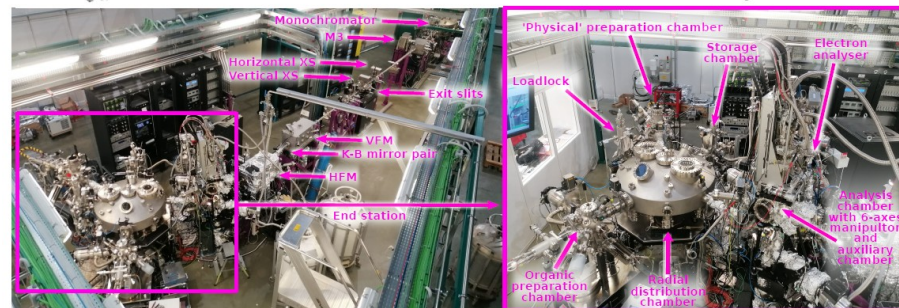
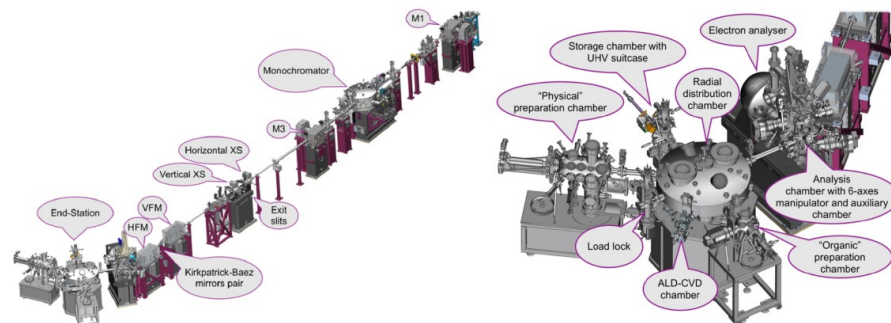
- 6 axes of movement.
- Allows reaching temperatures lower than 7.5 K .



Experimental methods



LOREA beamline



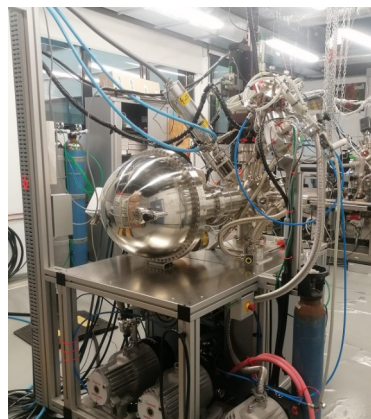
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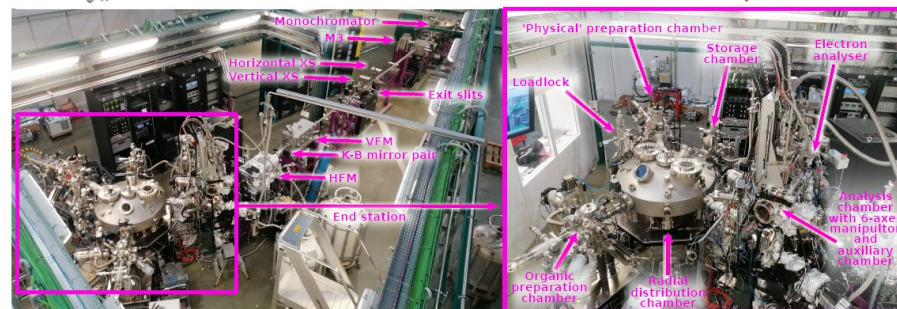
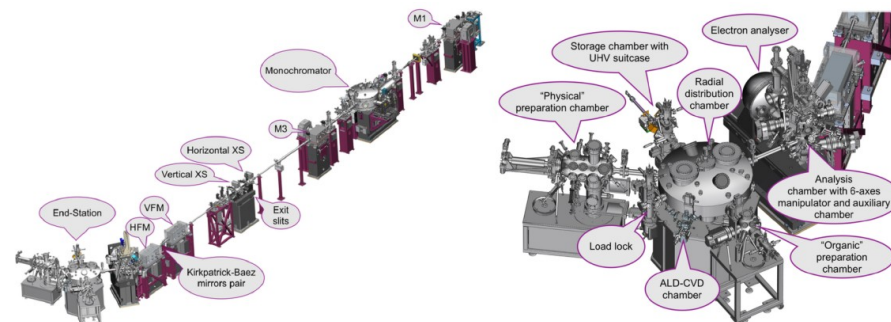
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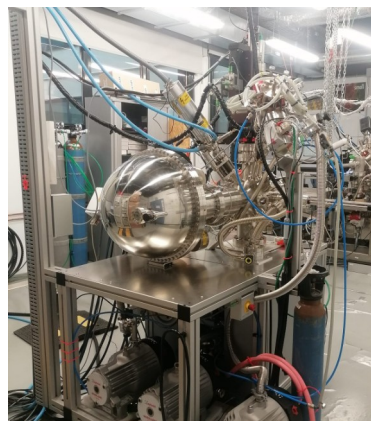


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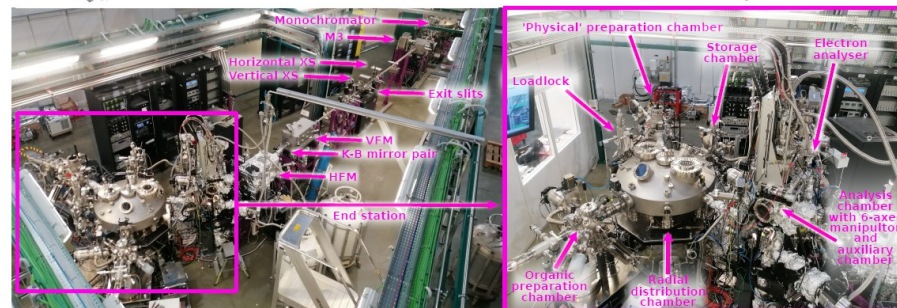
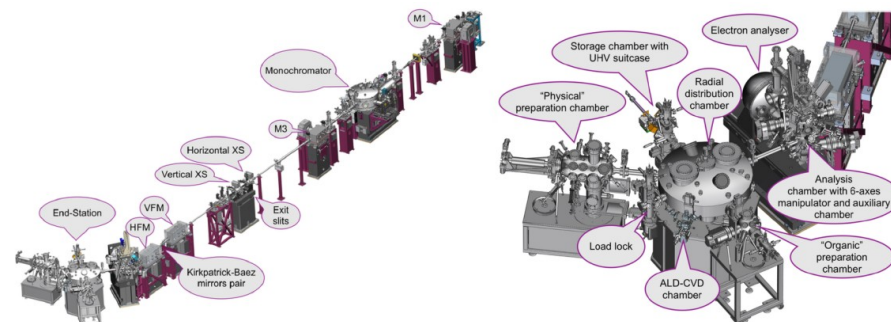
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- **Bulk single crystal**
- **Er impurities** deposited by means of an e-beam evaporator.
- XPS and ARPES performed at a **T = 15 K**
- **Exfoliated in-situ (UHV)** at T = 15 K
- **Linear horizontal polarization**
hν = 100 (XPS) and 52 (ARPES) eV

LOREA beamline

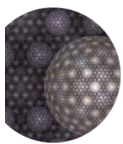


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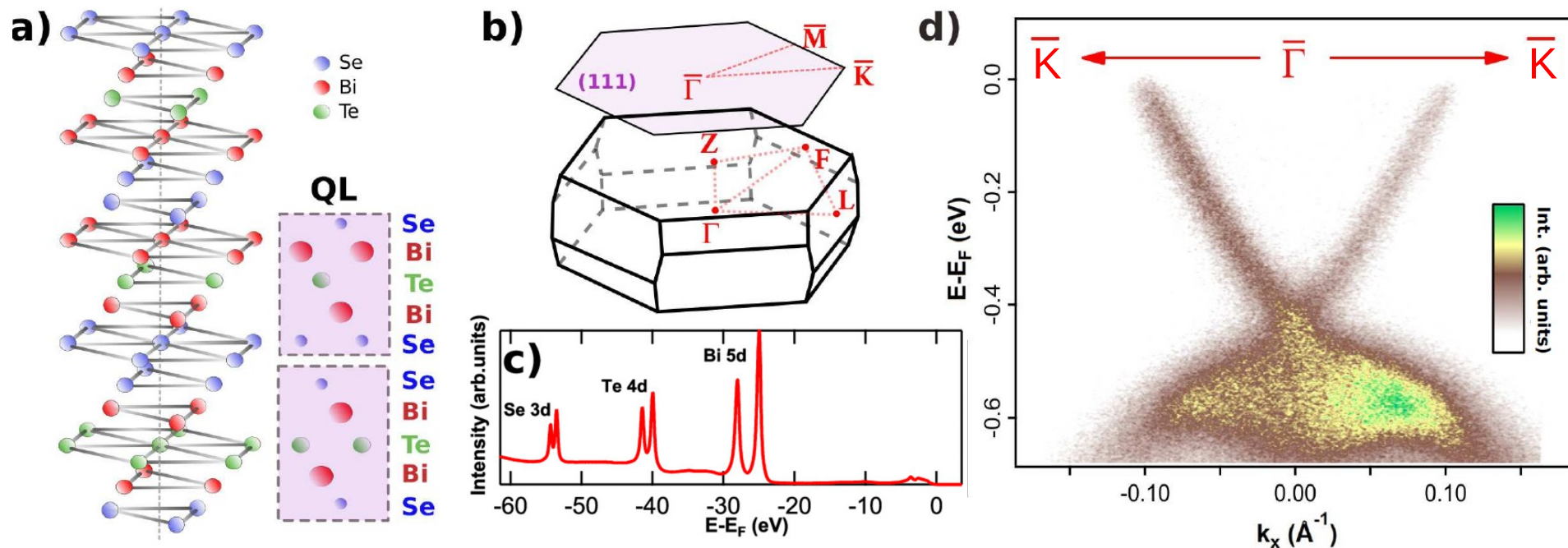
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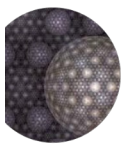
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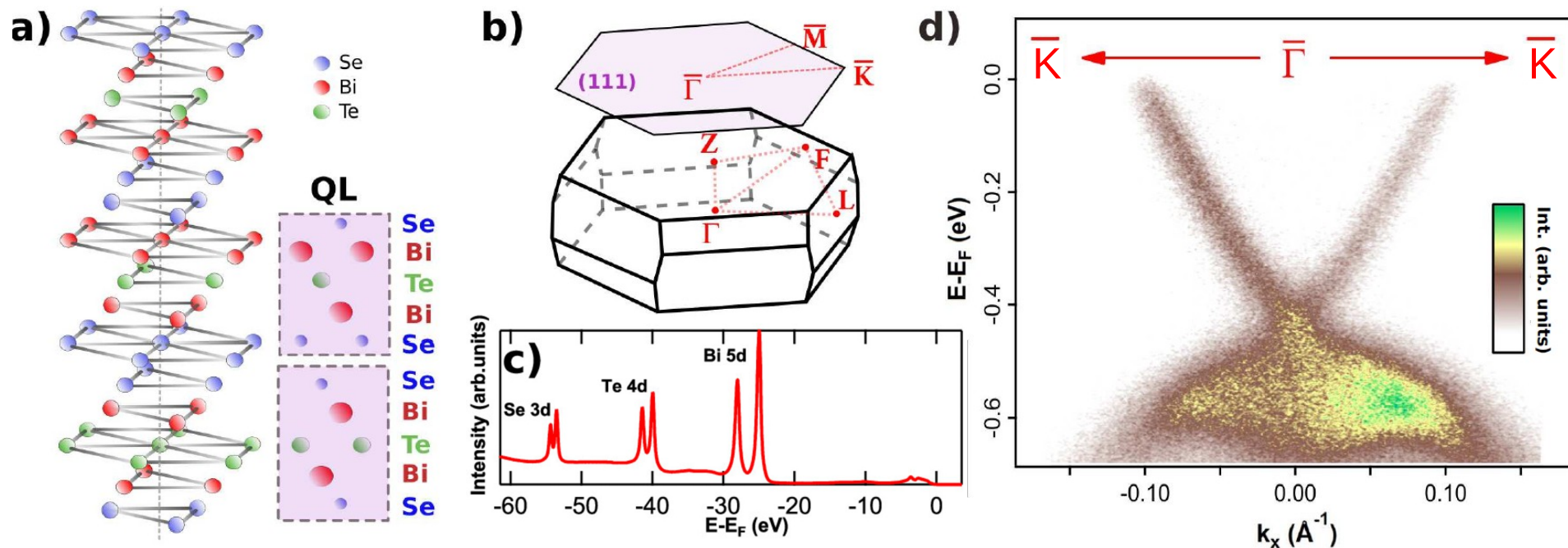


Results: pristine $\text{Bi}_2\text{Se}_2\text{Te}$

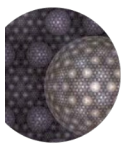




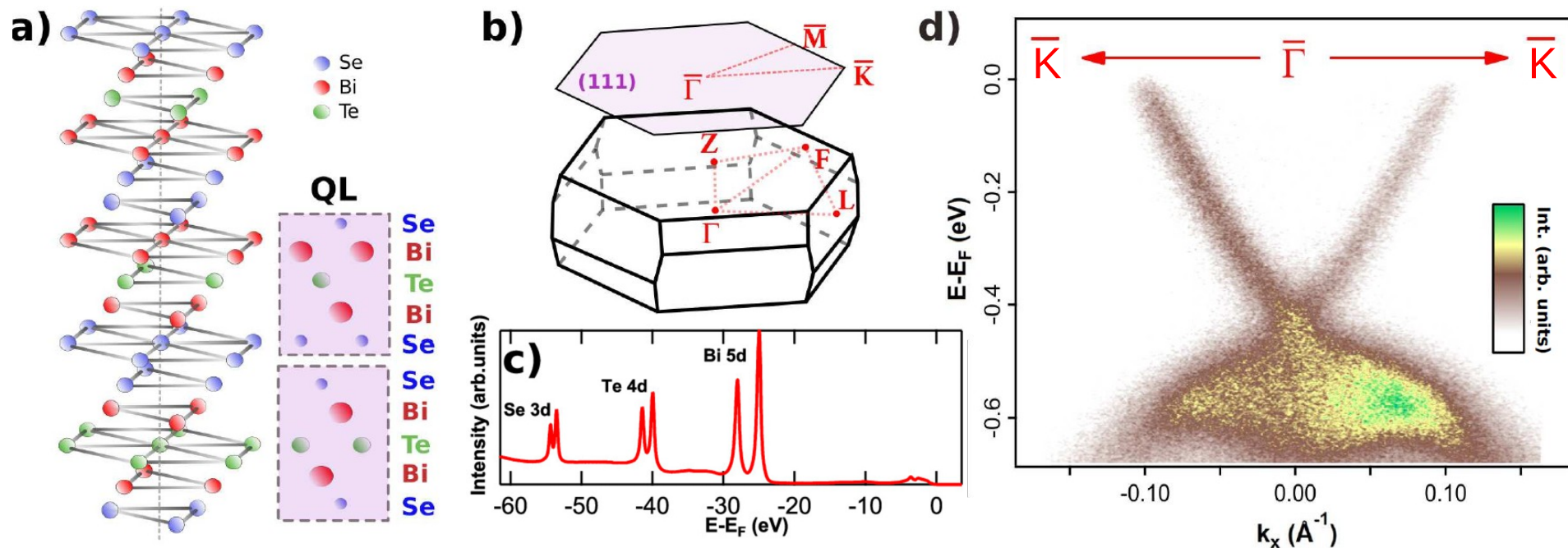
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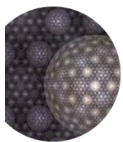
- 3D quintuple layer crystal structure.



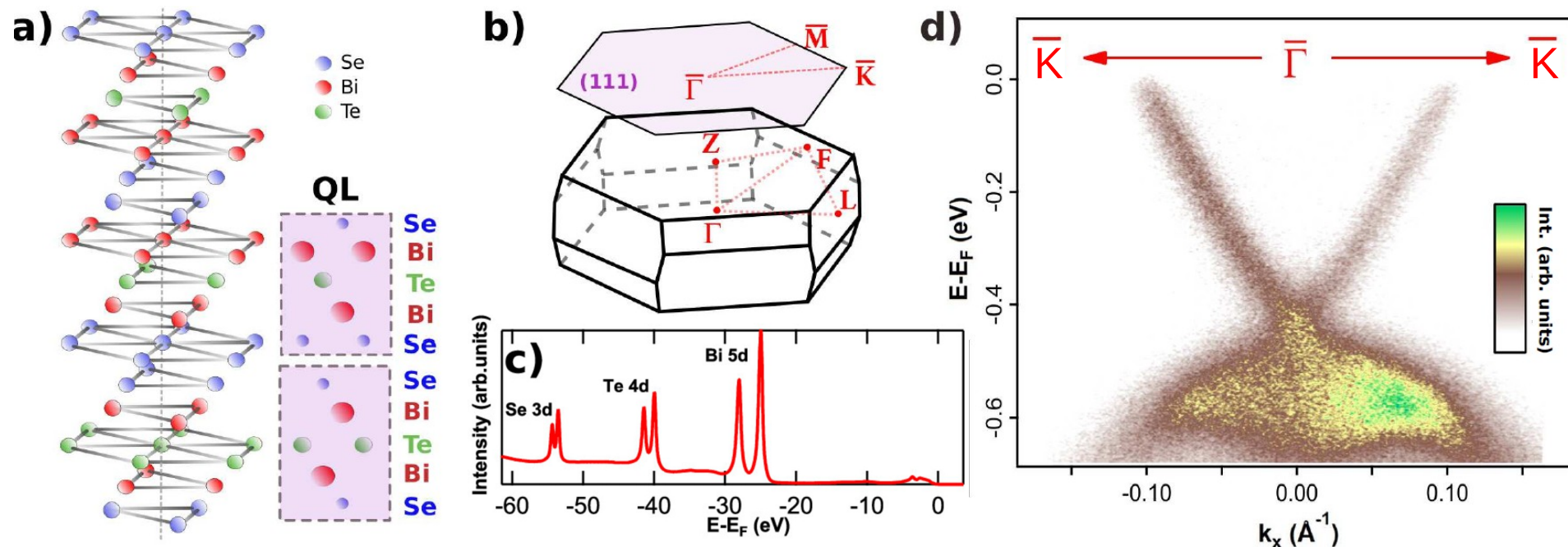
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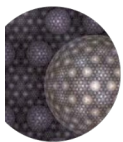
- 3D quintuple layer crystal structure.
- **Brillouin zone (BZ) and projected surface BZ of $\text{Bi}_2\text{Se}_2\text{Te}$.**



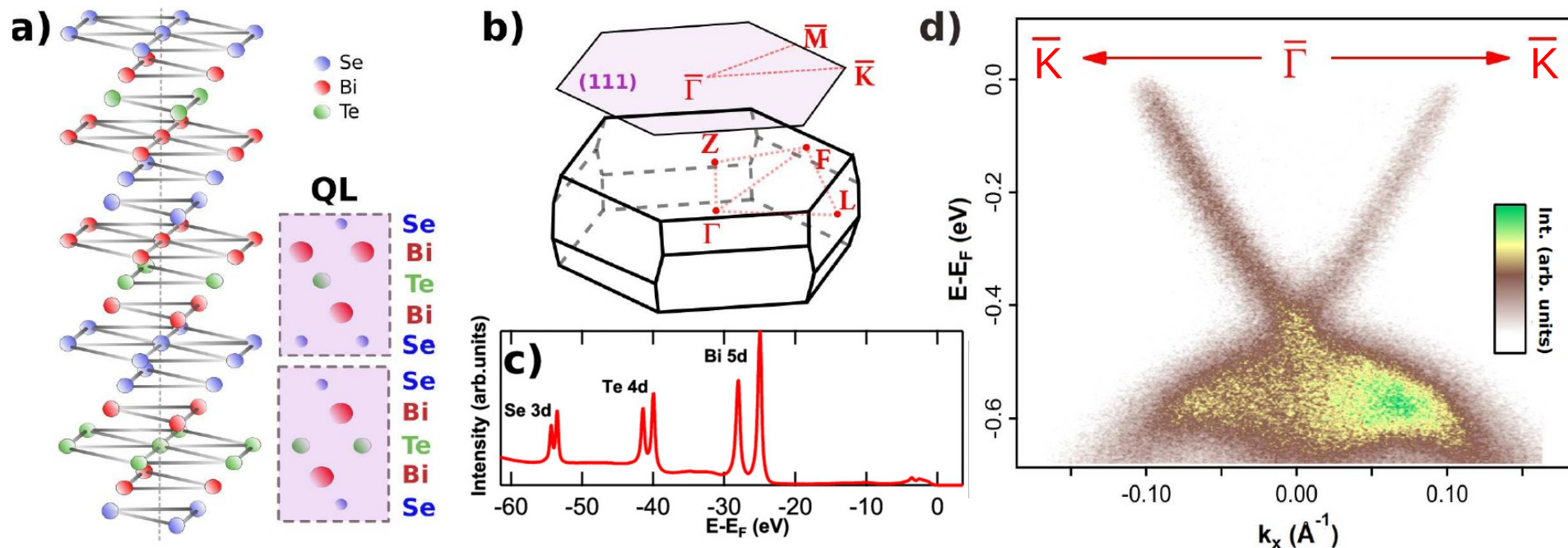
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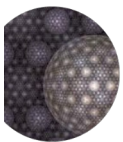
- 3D quintuple layer crystal structure.
- Brillouin zone (BZ) and projected surface BZ of $\text{Bi}_2\text{Se}_2\text{Te}$.
- **XPS spectrum: intense and narrow peaks**, very well defined **spin-orbit doublets** prove the **surface quality** after *in situ* exfoliation.



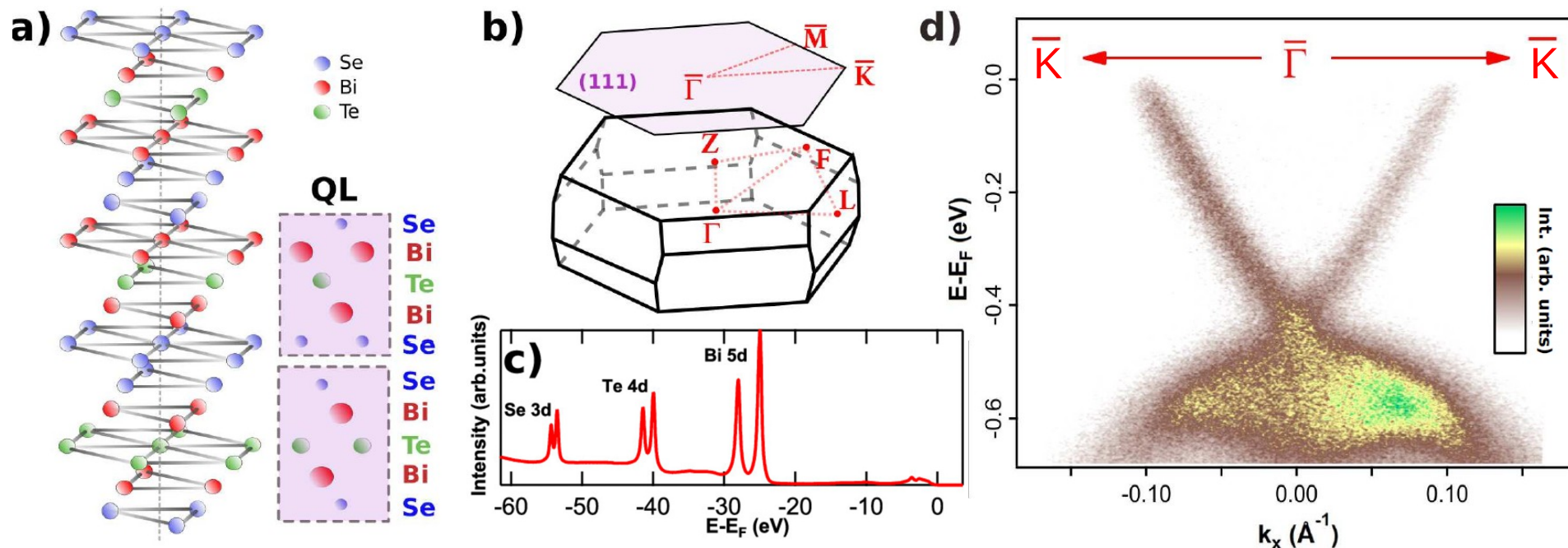
Results: pristine $\text{Bi}_2\text{Se}_2\text{Te}$



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- Pristine $\text{Bi}_2\text{Se}_2\text{Te}$ TSS **ARPES** bandmap along the $\Gamma\bar{K}$ direction **yields:**

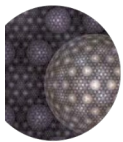


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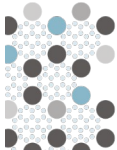


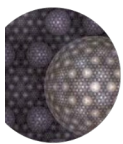
- 3D quintuple layer crystal structure.
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$$E_{\text{DP}} = 440 \text{ meV}$$
$$\text{No gap}$$
$$V_F = (7.1 \pm 0.1) \cdot 10^5 \text{ m/s}$$

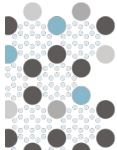
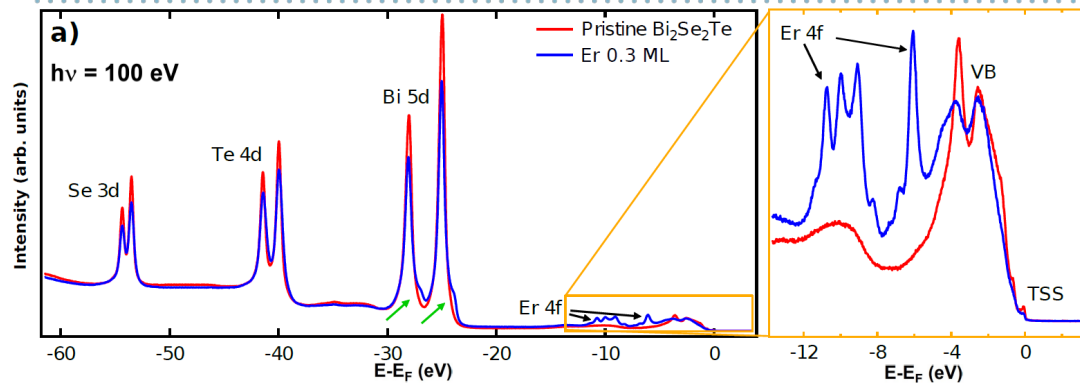


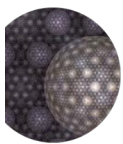
Results: Er-doped $\text{Bi}_2\text{Se}_2\text{Te}$ XPS



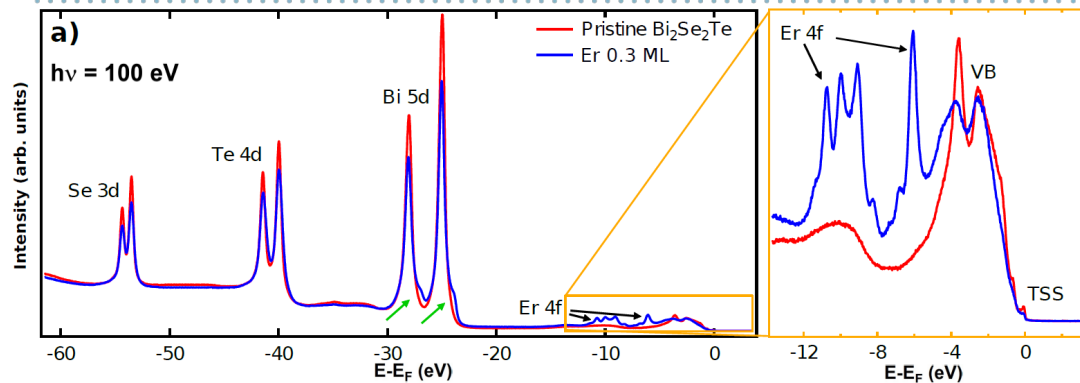


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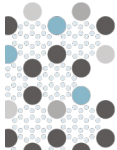


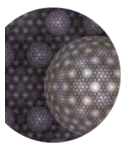


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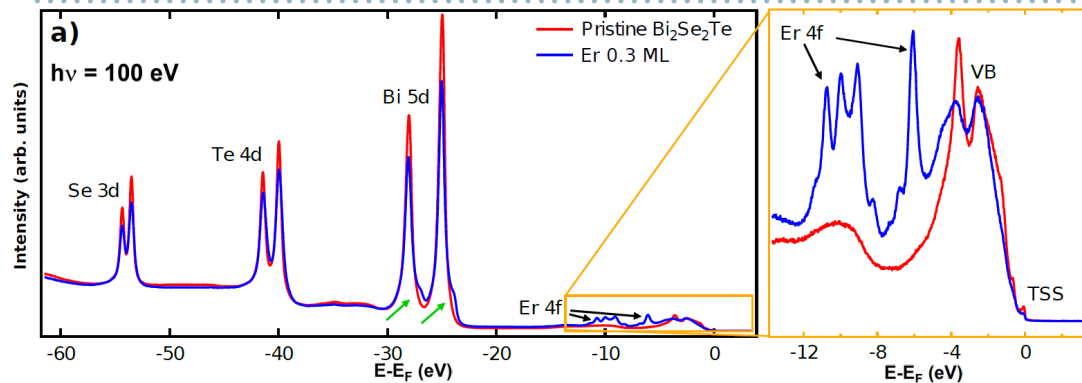


- Se 3d, Te 4d, Bi 5d → **attenuated**.

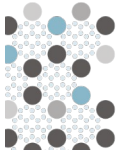


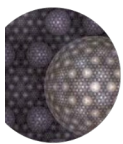


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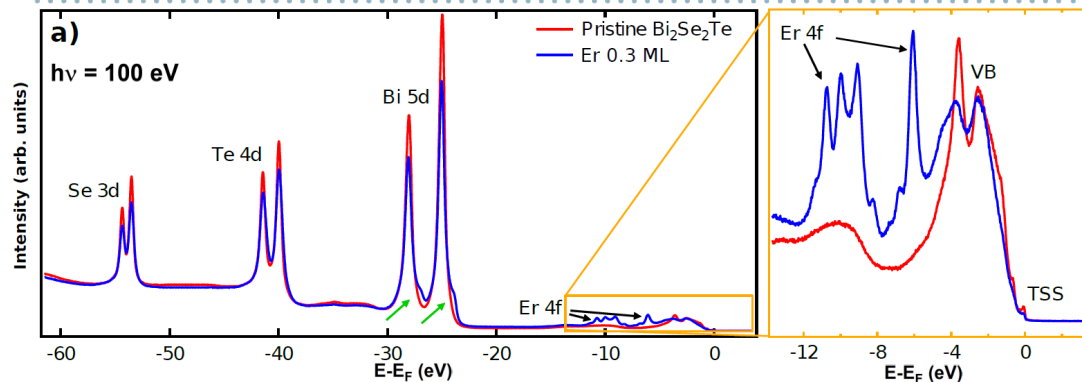


- Se 3d, Te 4d, Bi 5d → attenuated.
- No extra components at higher BEs → **no surface oxidation or contamination**

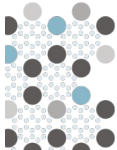


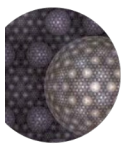


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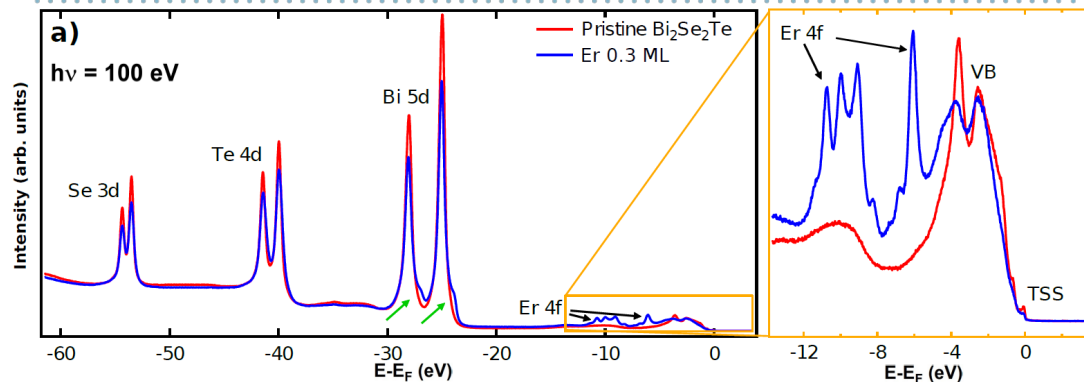


- Se 3d, Te 4d, Bi 5d → attenuated.
- No extra components at higher BEs → no surface oxidation or contamination
- No widening of the peak + very sharp and well resolved multippeak structure **Er 4f** states → **no further disorder introduced**

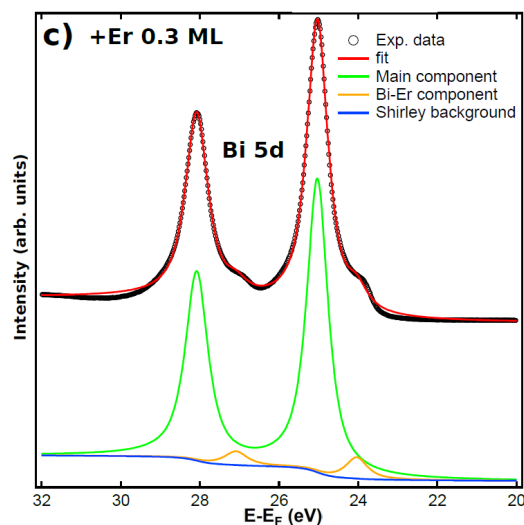
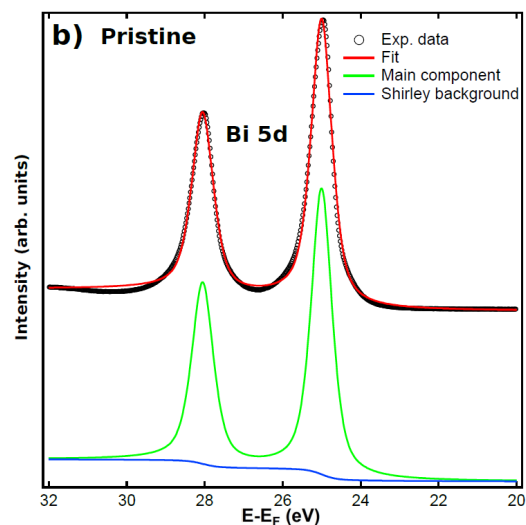


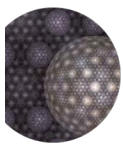


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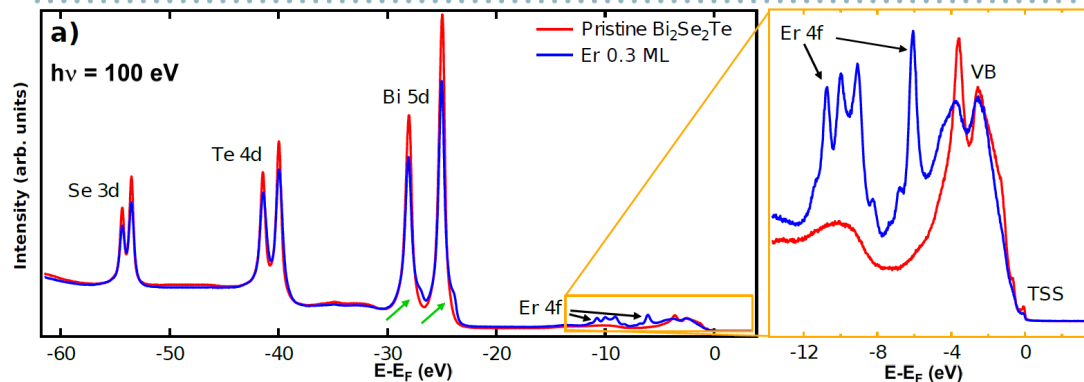


- Se 3d, Te 4d, Bi 5d $\rightarrow$ attenuated.
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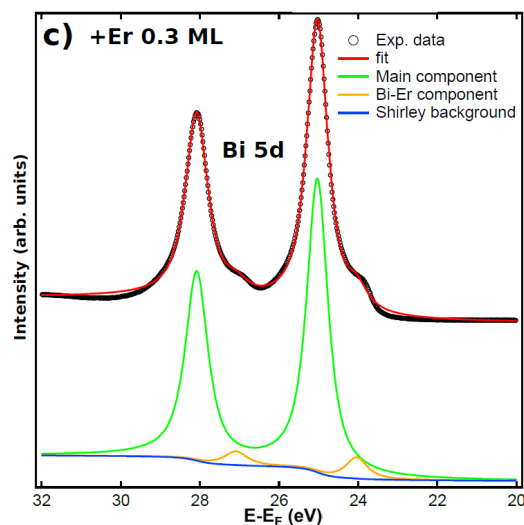
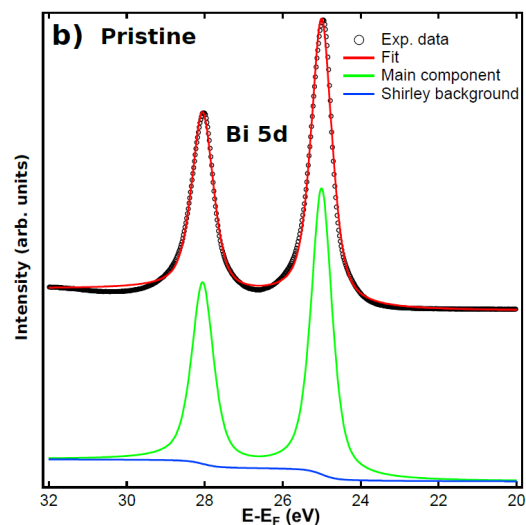


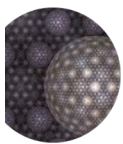


Results: Er-doped $\text{Bi}_2\text{Se}_2\text{Te}$ XPS

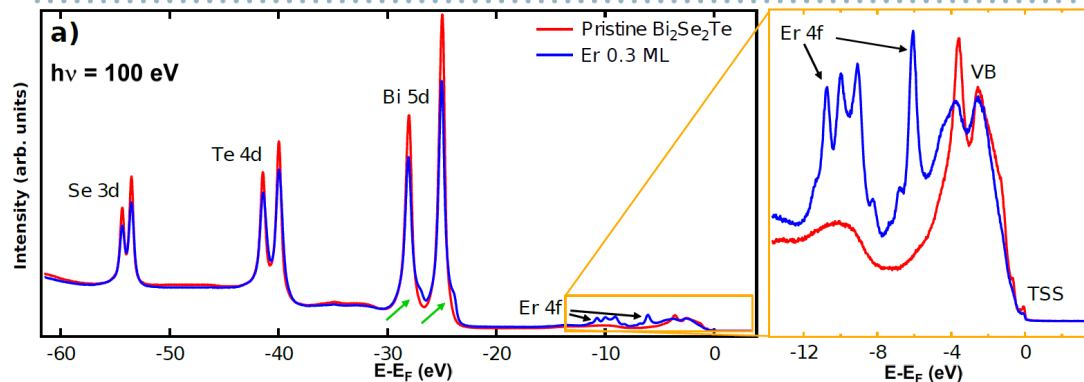


- Se 3d, Te 4d, Bi 5d $\rightarrow$ attenuated.
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- **Second Bi 5d component** $\rightarrow$ intensity linearly increases with the Er coverage $\rightarrow$ related to superficial **Bi-Er bond** + interaction at the RE-TI interface

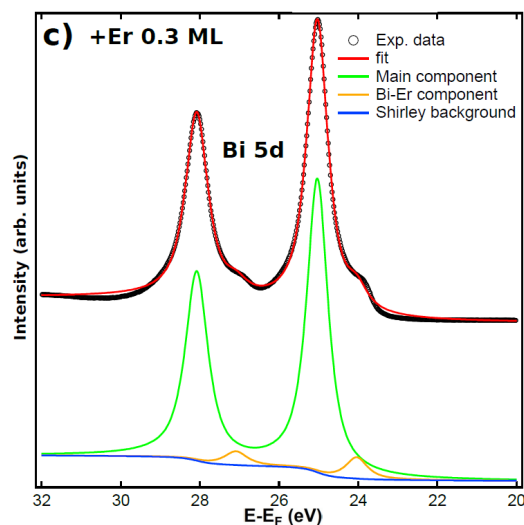
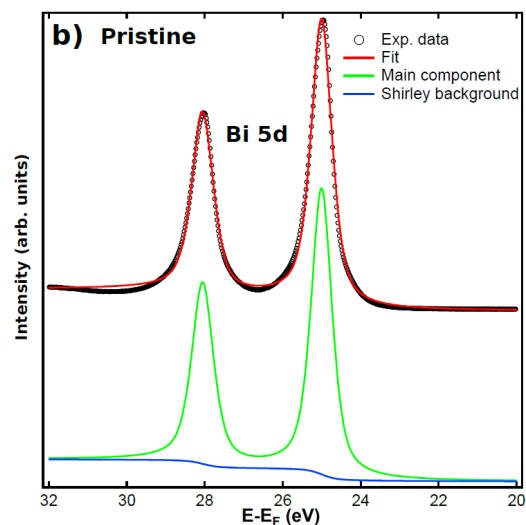




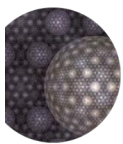
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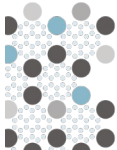
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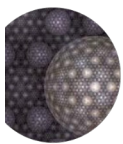


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- Bi 5d peak attenuation $\rightarrow$ **Er coverage estimation**



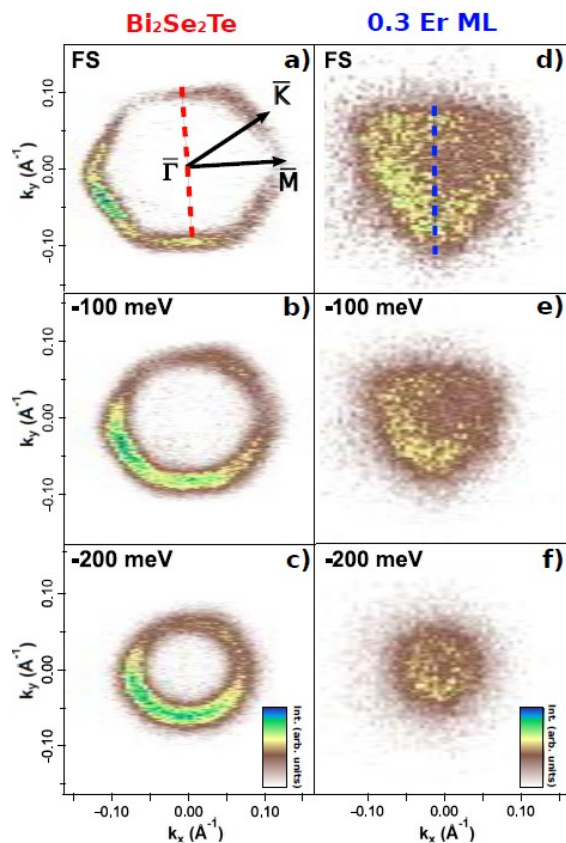
Results: pristine vs. Er-doped $\text{Bi}_2\text{Se}_2\text{Te}$ Fermi maps

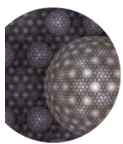




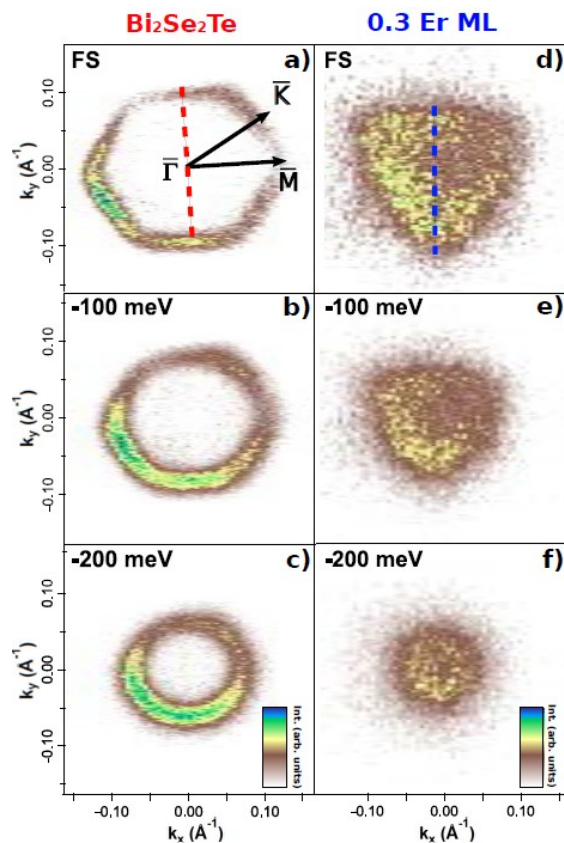
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- **Pristine BST TSS** → **hexagonal warped FS** and the circular CE maps.

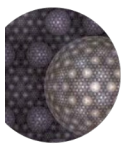




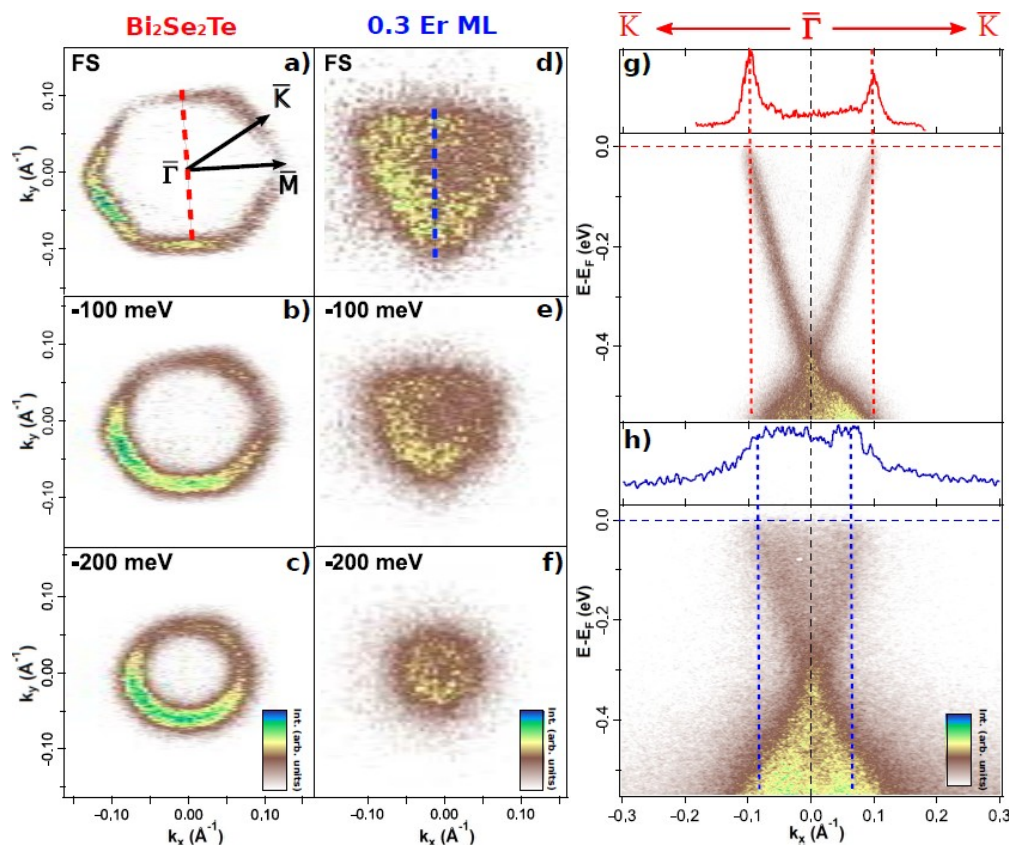
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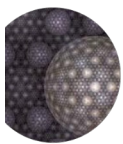
- Pristine BST TSS → hexagonal warped FS and the circular CE maps.
- **Er-doped** BST TSS → TSS warping symmetry: **hexagonal → trigonal**



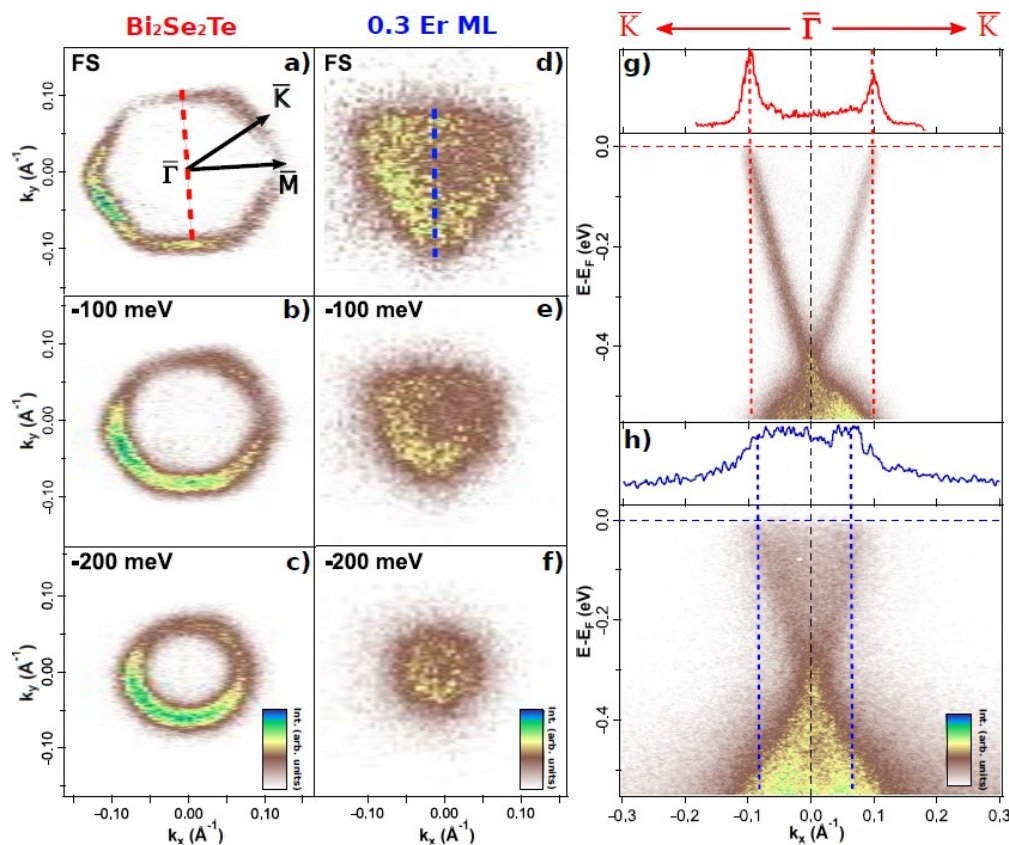
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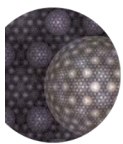
- Pristine BST TSS $\rightarrow$ hexagonal warped FS and the circular CE maps.
- Er-doped BST TSS $\rightarrow$ TSS warping symmetry: hexagonal $\rightarrow$ trigonal
- **Induced inversion asymmetry in the TSS** band dispersion in along the ΓK direction



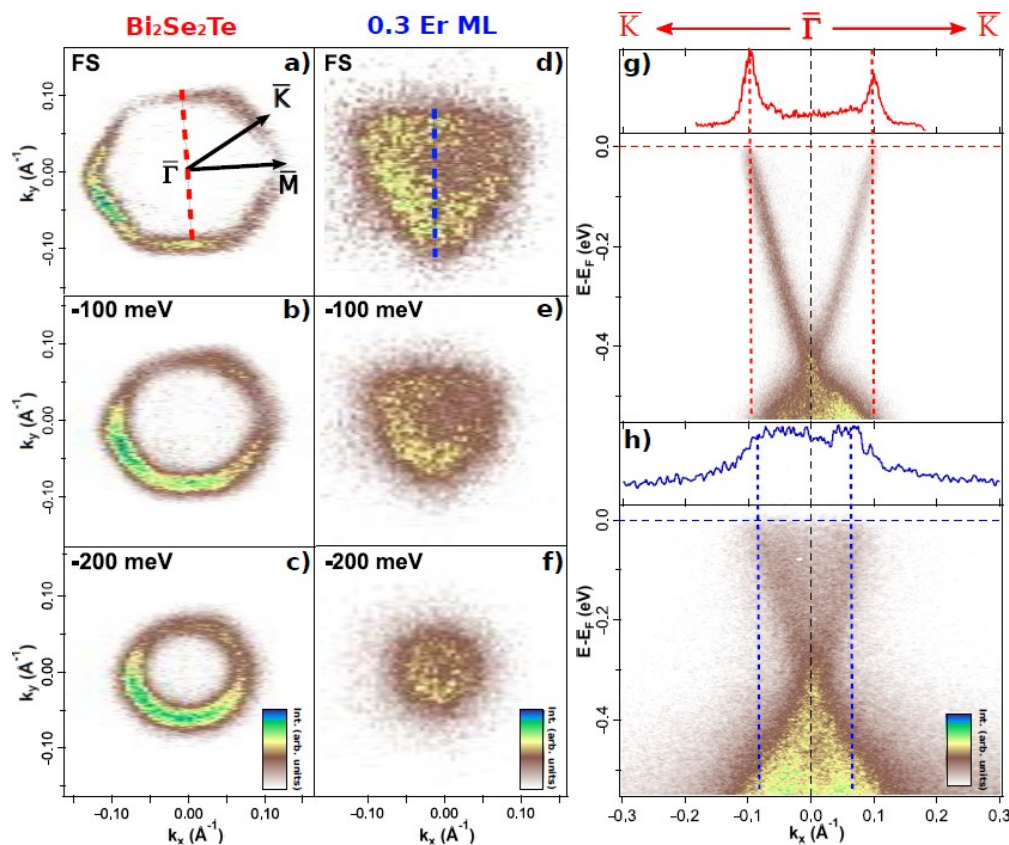
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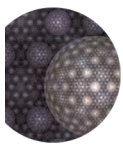
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 - MDCs along dashed lines
 - **Pristine $\text{Bi}_2\text{Se}_2\text{Te}$:**
same branch $v_F \rightarrow$ **symmetric k_F**



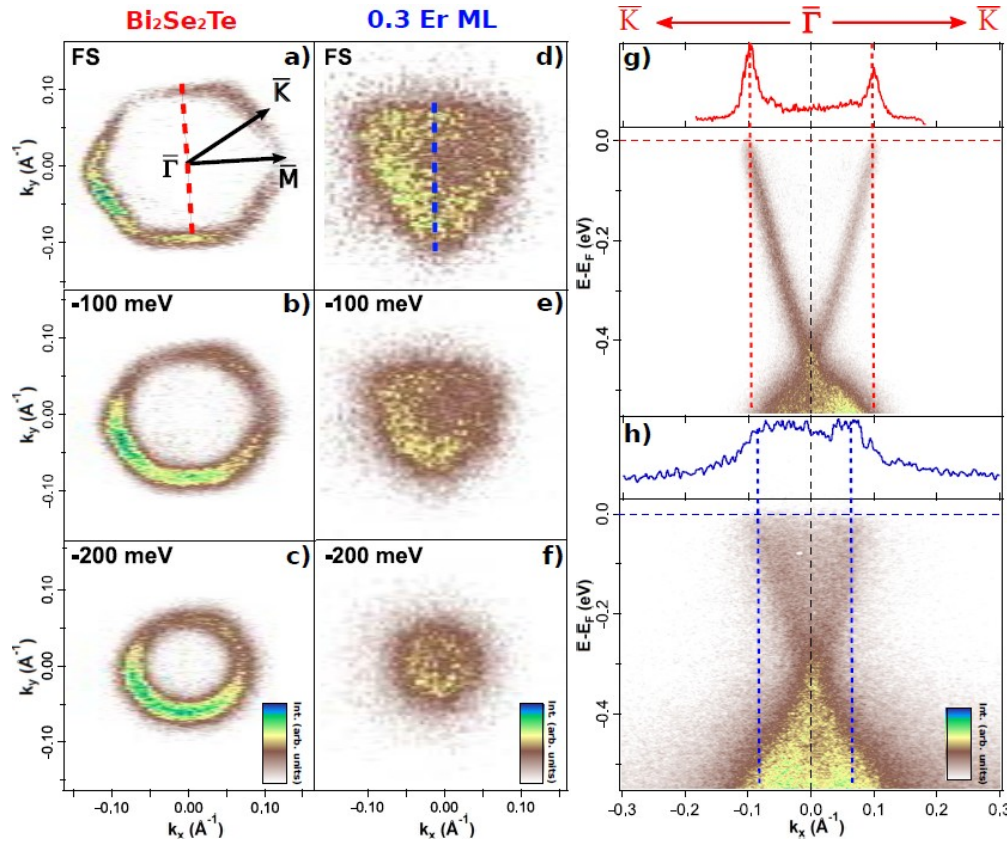
Results: pristine vs. Er-doped $\text{Bi}_2\text{Se}_2\text{Te}$ Fermi maps



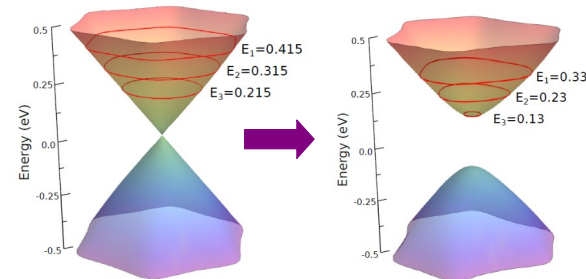
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 - Pristine $\text{Bi}_2\text{Se}_2\text{Te}$: same branch $v_F \rightarrow$ symmetric k_F
 - **Er-doped $\text{Bi}_2\text{Se}_2\text{Te}$:** different branch $v_F \rightarrow$ **asymmetric k_F**



Results: pristine vs. Er-doped $\text{Bi}_2\text{Se}_2\text{Te}$ Fermi maps

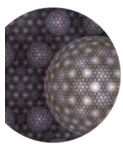


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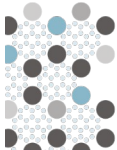


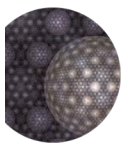
- Theoretical model $\rightarrow$ magnetic Zeeman out-of-plane term in Hamiltonian

$$H = \hbar v_F (k_x \sigma_y - k_y \sigma_x) + (\lambda k^3 \cos 3\theta - \Delta) \sigma_z$$

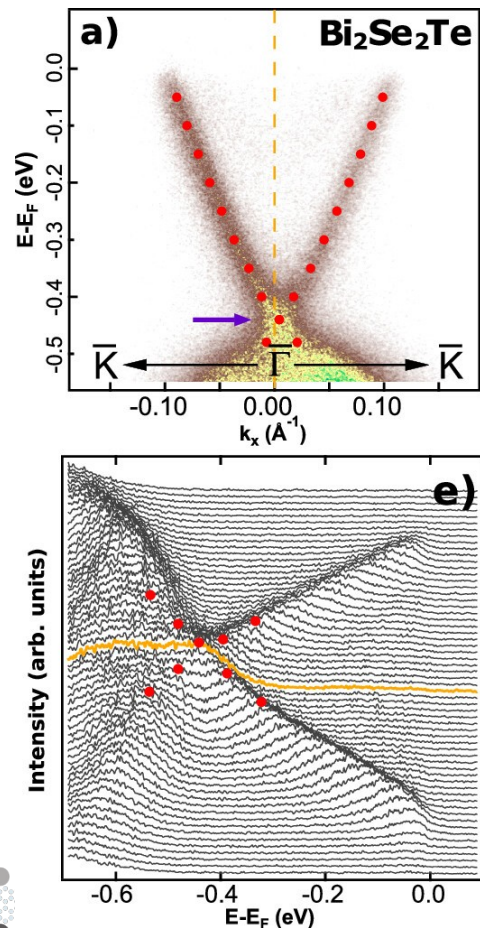


Results: bandgap opening at the Dirac point

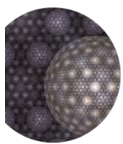




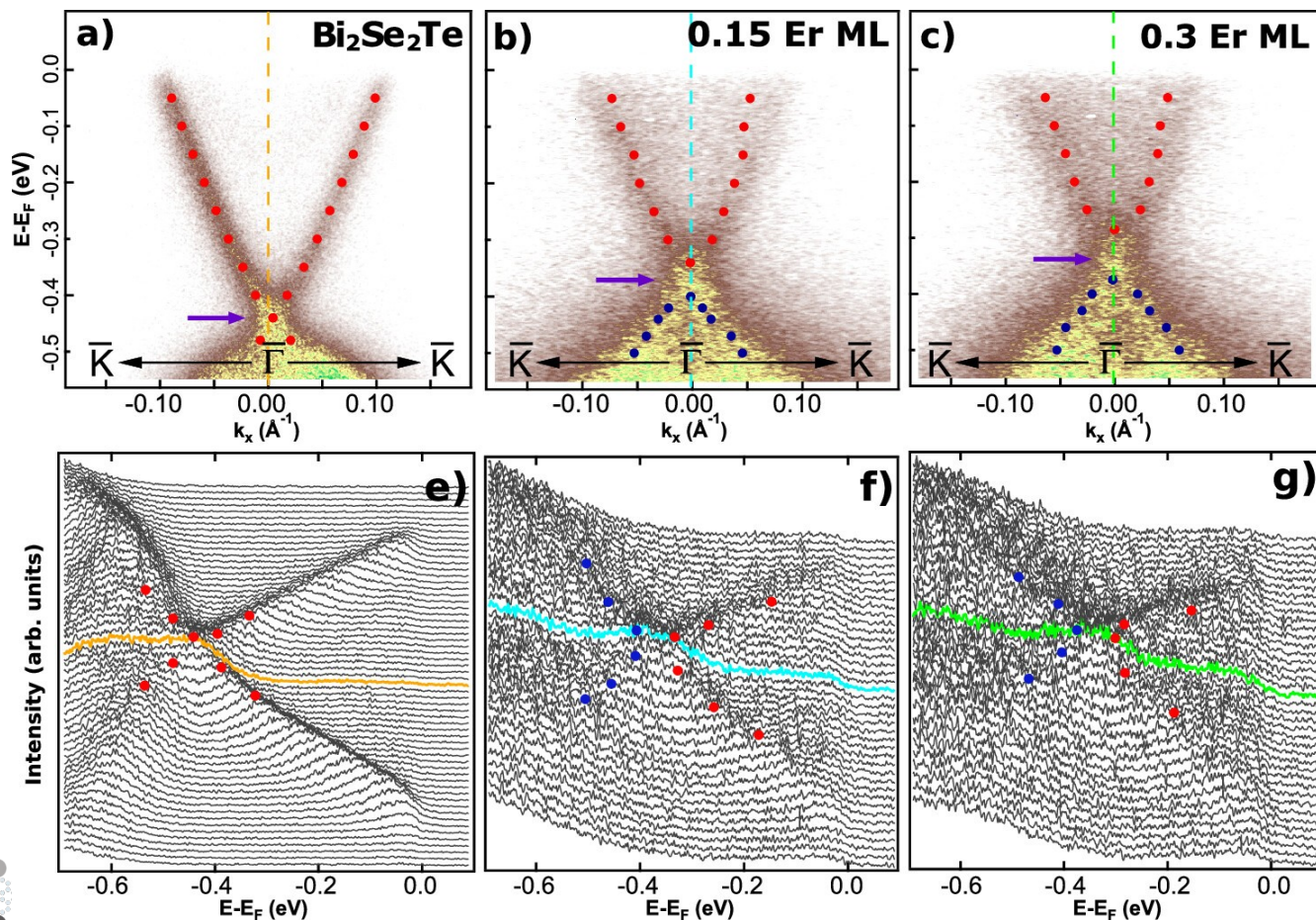
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- **Pristine BST:**
 - **DP defined** as intersection of two linear branches at 440 meV
 - **Punctual maximum** of intensity in the EDC at Γ

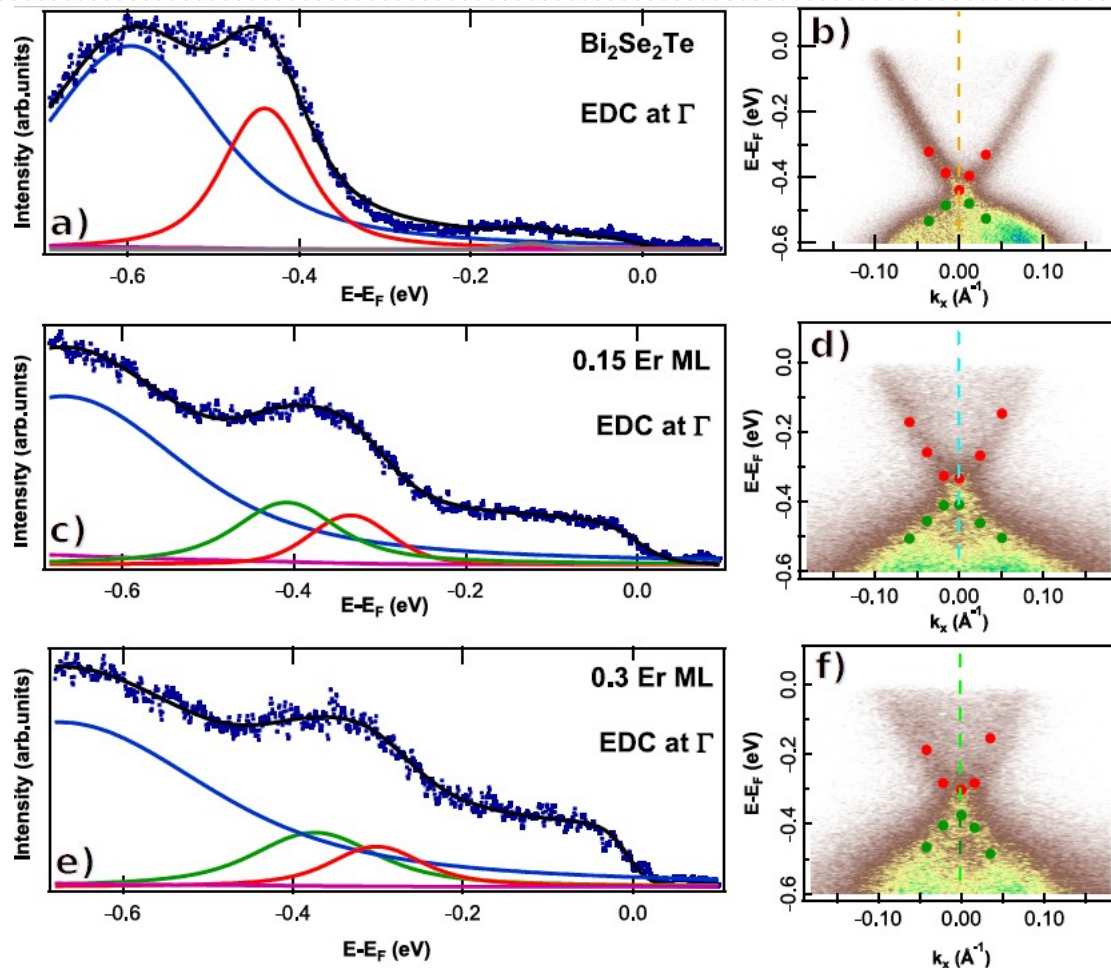


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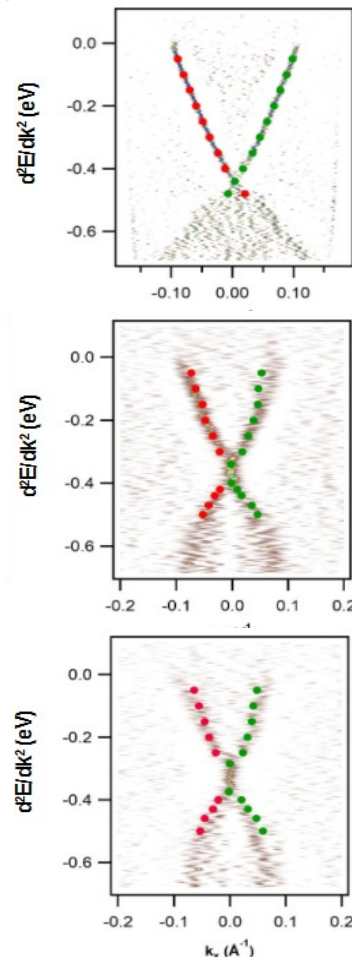
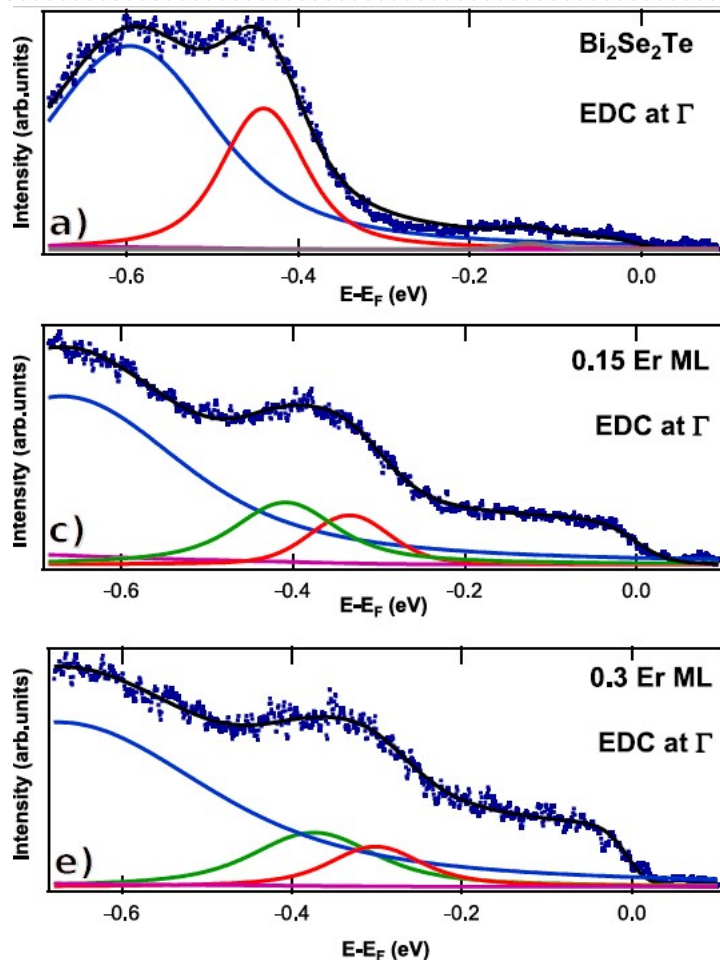
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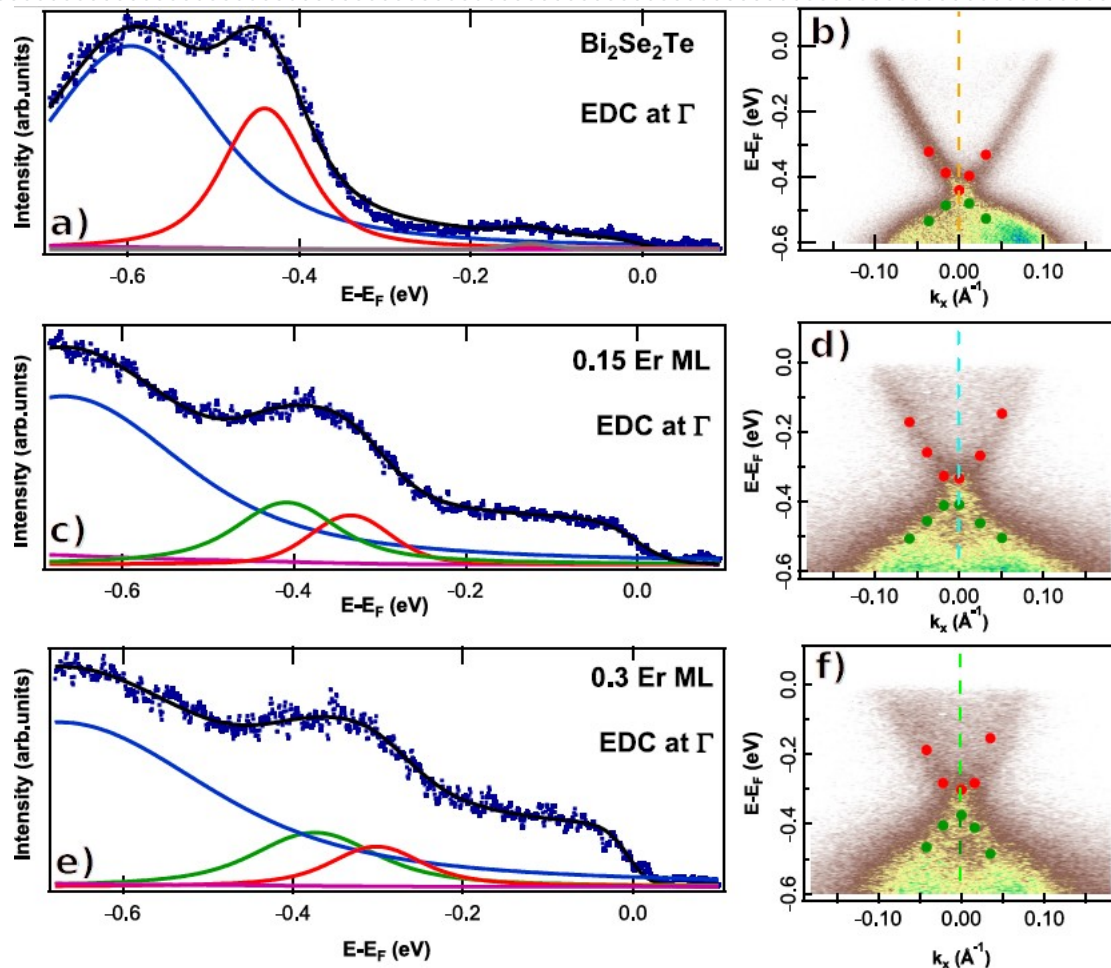
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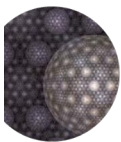
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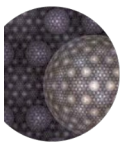
Gap opening



Summary and conclusions

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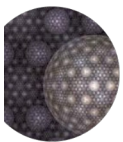




Summary and conclusions

- Prototypical 3D TI $\text{Bi}_2\text{Se}_2\text{Te}$ magnetically doped with low concentrations of Er

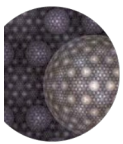




Summary and conclusions

- Prototypical 3D TI $\text{Bi}_2\text{Se}_2\text{Te}$ magnetically doped with low concentrations of Er
- **Firts experimental observation** of the magnetically induced **transition** of the **warping** of the TSS from hexagonal to trigonal

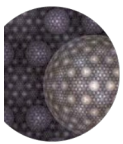




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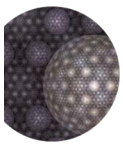




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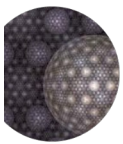




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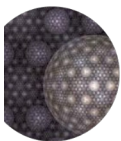




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- **Controlled doping of TIs with REs** as an excellent approach to realize the **QAHE** **at higher temperatures** since it fulfills all its requirements





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Pierre A. Pantaleón
Jose Angel Silva-Guillén

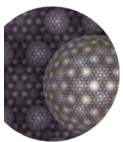
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Aitor Mugarza



BL20 – LOREA
Ji Dai
Massimo Tallarida





Thank you!



