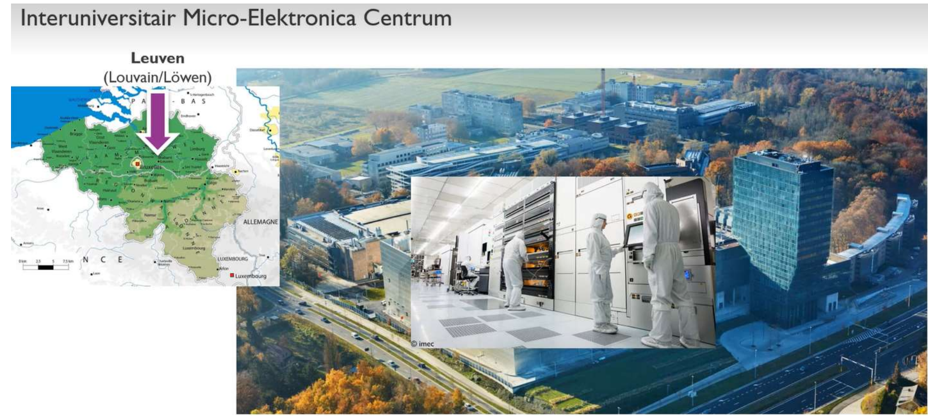


imec

CHARACTERIZATION OF 2D MATERIALS BY ARPES AT IMEC

PRESENTED BY PAUL VAN DER HEIDE

Dhirendra Pratap Singh, Fabian Holzmeier, Kevin Dorney, Esben Witting Larsen, Thierry Conard, John Petersen

AGENDA

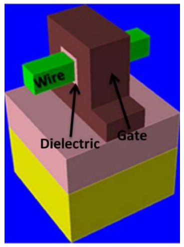
What next : 2D materials-Beyond CMOS

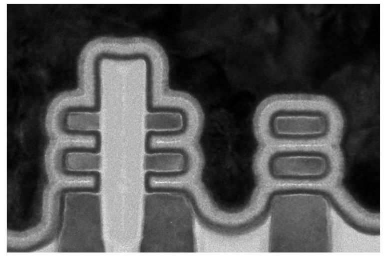
Photo Emission techniques

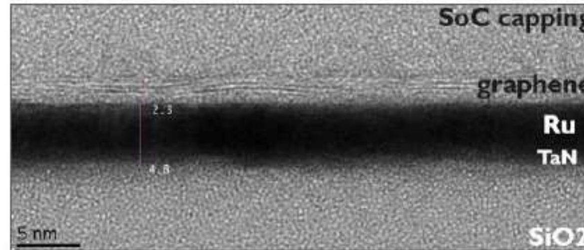
The imec AttoLab

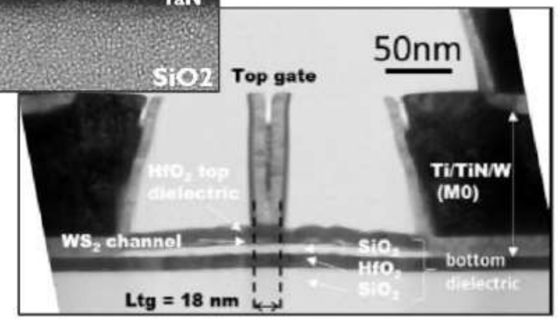
Results

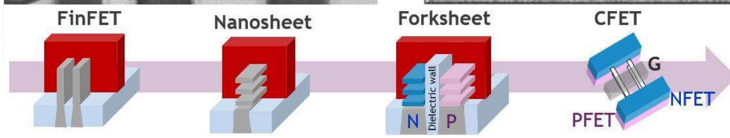
WHAT NEXT





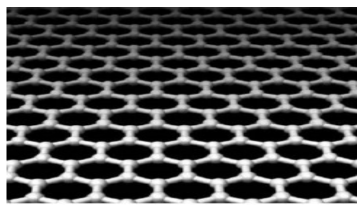


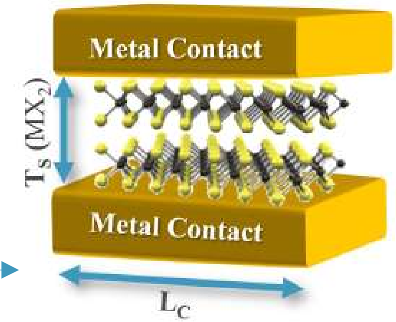


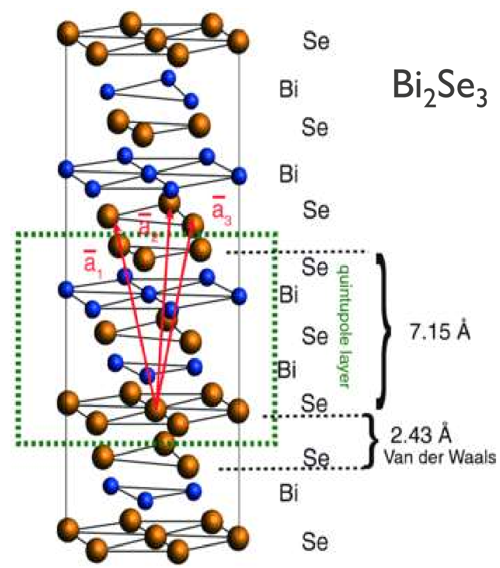


- Continued scaling:
  - Logic: FinFET, GAA, CFET →
  - Memory: ReRAM, PCRAM, MRAM, 3D-DRAM, …

- And then?
  - 2D Materials?
    - Graphene →
    - Transition Metal Dichalcogenides (TMD) →
    - 3D Topological Insulators (2D & 3D-TIs) →



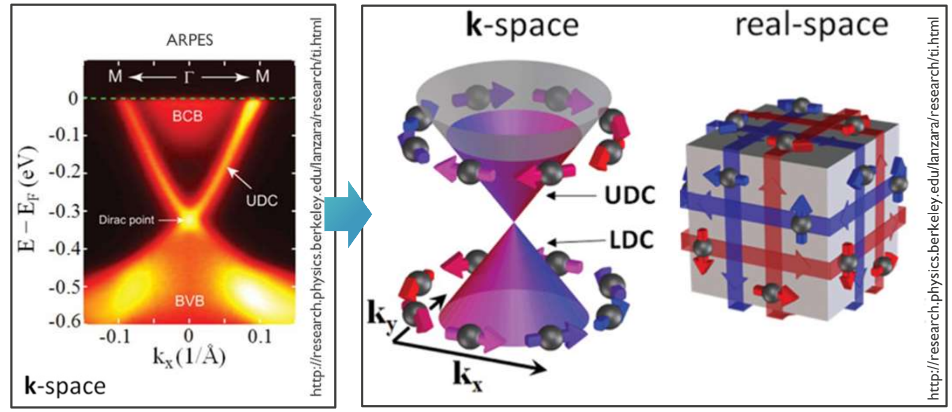




- How can a 3D-TI be a 2D material
  - Conduction only occurs along the surface of these insulators

Semicond. Sci. Technol. 27 (2012) 124001

TOPOLOGICAL INSULATORS



ARPES=Angle Resolved Photo Electron Spectroscopy

- TI chronology
  - 2005: 1st theorized
  - 2007: 1st verified (via ARPES)

A new electronic phase

- Why are TIs important
  - Charge carriers are spin polarized and immune to scattering (no leakage)
    - Potential applications include Spintronics inclusive of Quantum computing

New computing architectures

- Where do TI properties stem from
  - The Quantum Spin Hall Effect (QSHE)
    - QSHE is a result of Spin Orbit Splitting (SOS) analogous to the Quantum Hall Effect (QHE)

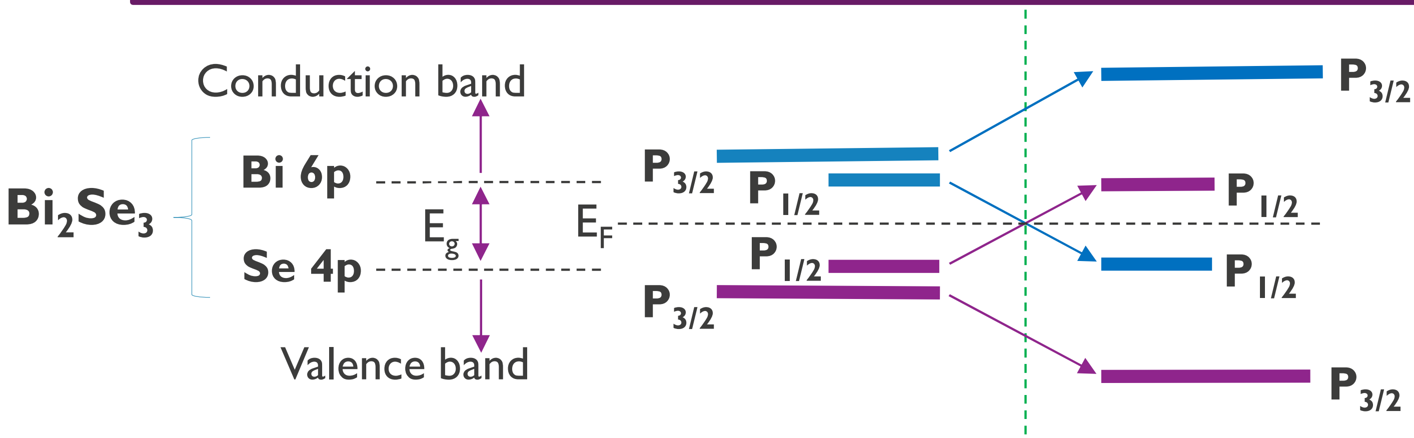
QHE=Quantum Hall Effect
QSHE=Quantum Spin Hall Effect

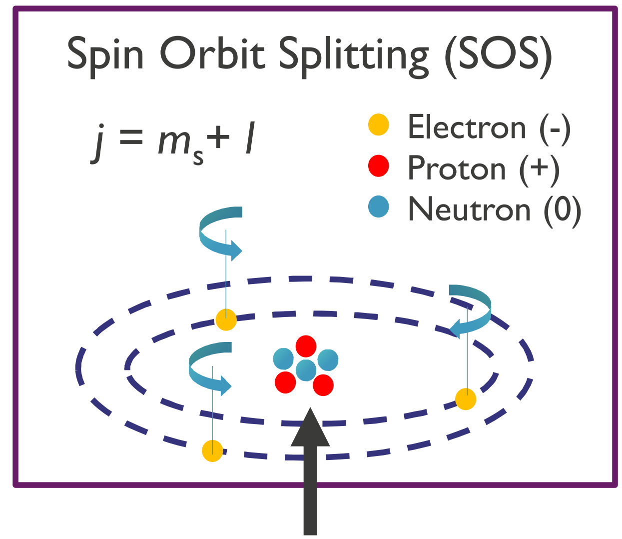
2016 Nobel prize in physics

QHE & QSHE

- Impact of magnetic fields on band structure (external=QHE or internal (SOS)=QSHE)

QHE	Zero B	Medium B	High B
QSHE	Insulator	Interface	3D TI (bulk insulator)





Spin of nucleus (protons) effects SOS

Level crossing (parity allowed)

Results in conduction at Localized Surface States (LSS)

Computing at the interface ?

AGENDA

What next : 2D materials-Beyond CMOS

Photo Emission techniques

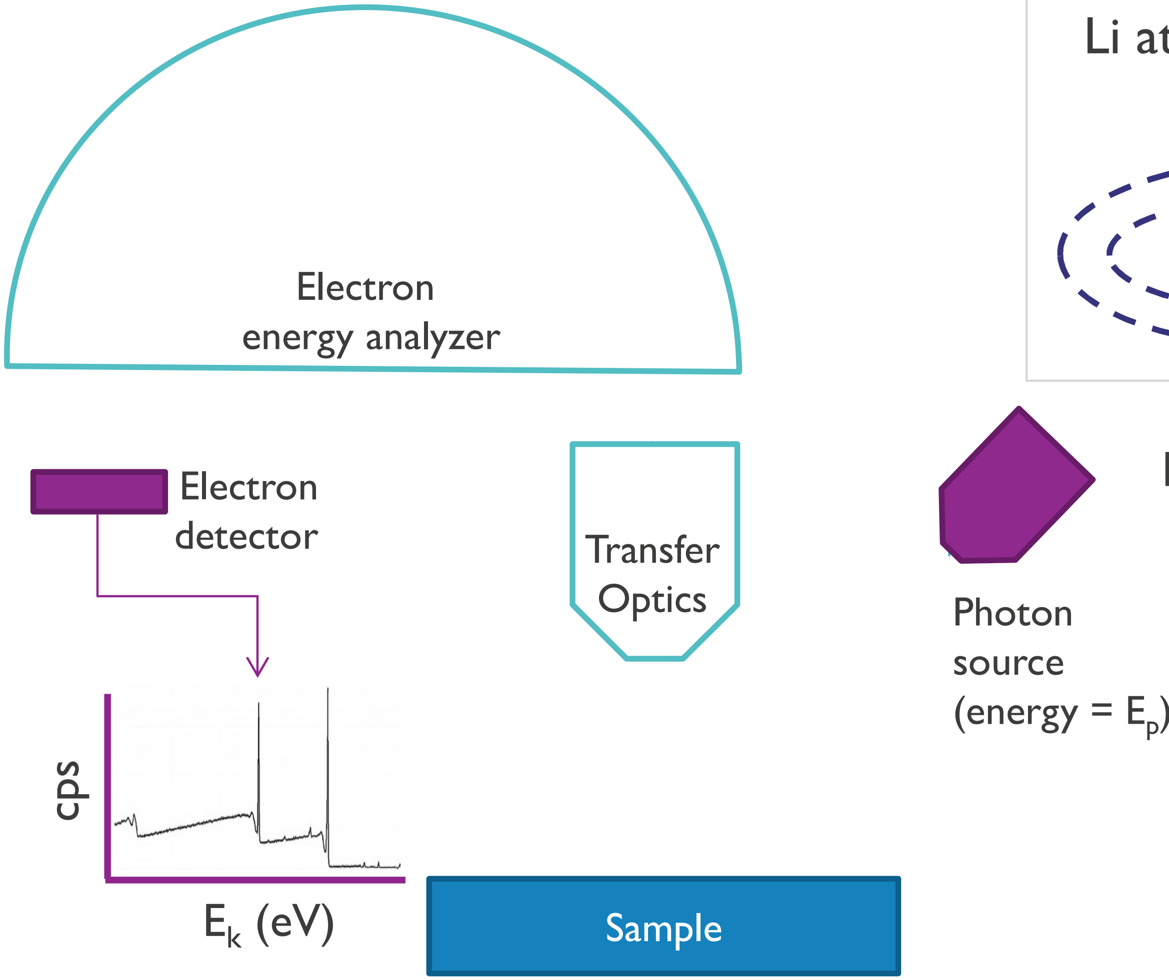
The imec AttoLab

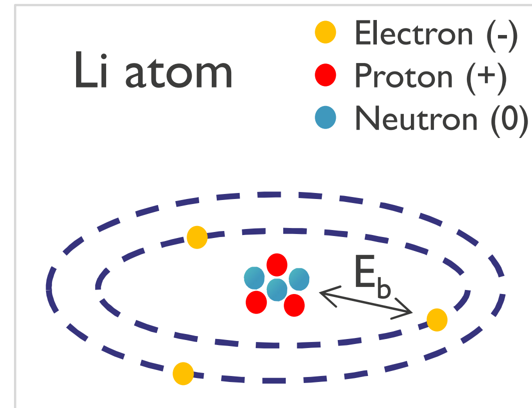
Results

ESCA=Electron Spectroscopy for Chemical Analysis
XPS=X-ray Photoelectron Spectroscopy
PES=Photo Emission Spectroscopy

FOR CORE LEVEL ANALYSIS

- Photons directed at solid sample. Photoelectrons recorded.
- Provides
  - Composition
  - Speciation
- Attributes
  - Non-destructive
  - Li-U detectable
  - DL: 0.1%





Photoelectron Kinetic energy (E_k) relates to Binding energy (E_b) via

$$E_p = E_k + E_b + \phi$$

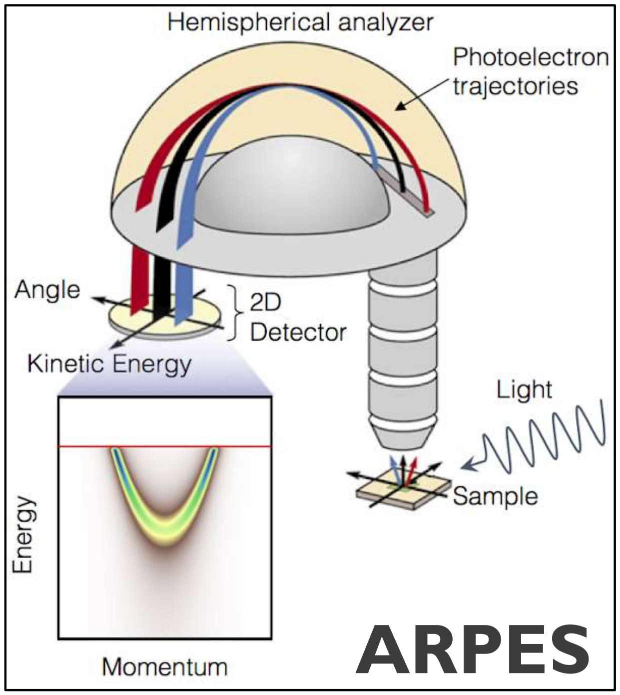
ϕ=Constant (instrument)

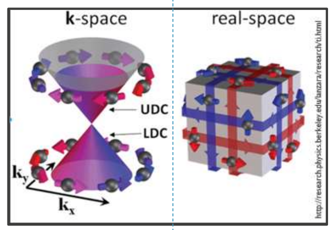
ARPES=Angle Resolved Photo Emission Spectroscopy
PEEM=Photo Electron Emission Microscopy
UPS=Ultra-violet Photoelectron Spectroscopy

FOR VALENCE BAND ANALYSIS

ARPES

- Maps the electronic band structure in *k-space*



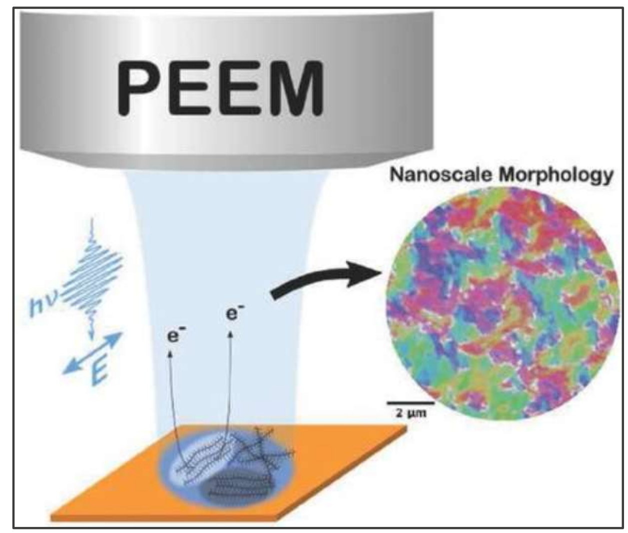


ARPES and PEEM are carried out in the same instrument using the same sources.

Analyzer settings differentiates the two.

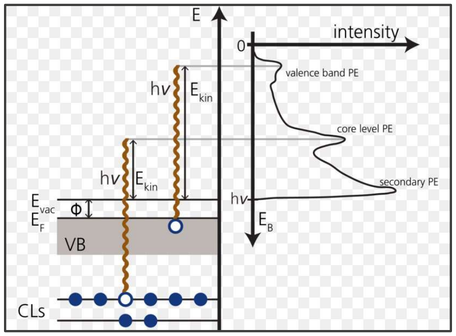
PEEM

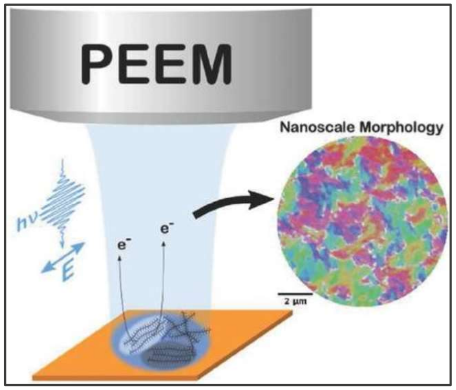
- Maps the surface of interest in *real-space*
  - Can be a specific E level or E band/s, i.e., recording E_F provides work-function map of surface

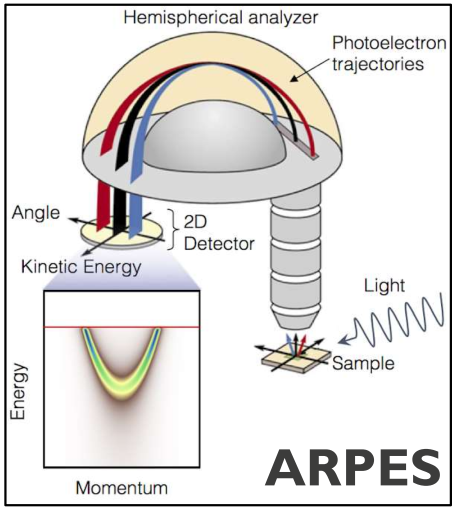


XPS-UPS-ARPES-PEEM

- All are Photo-Emission Spectroscopy (PES) techniques, but with different information content.







	Source*	Energy*	Levels	Extraction	Information
XPS/ ESCA	Al-kα* Synchrotron	1486.6 eV* Variable	Core	Zero to minimal (B)	Composition, elemental speciation + imaging to 2-10 µm in real space
PEEM	He-discharge*, Sync, HHG	21.22 eV*, Variable	Valence	High field (10 kV)	Spatial imaging to sub 100 nm in real space (20 nm optimal)
ARPES	He-discharge*, Sync, HHG	21.22 eV* Variable	Valence	High field (10 kV)	Electronic band structure (LUMO) in k space (also called momentum space)
UPS	He-discharge*, Sync, HHG	21.22 eV* Variable	Valence	Zero to minimal (B)	Electronic band structure (LUMO)/Density of States (DoS) in real space

* Refers to most commonly used source in industry

AGENDA

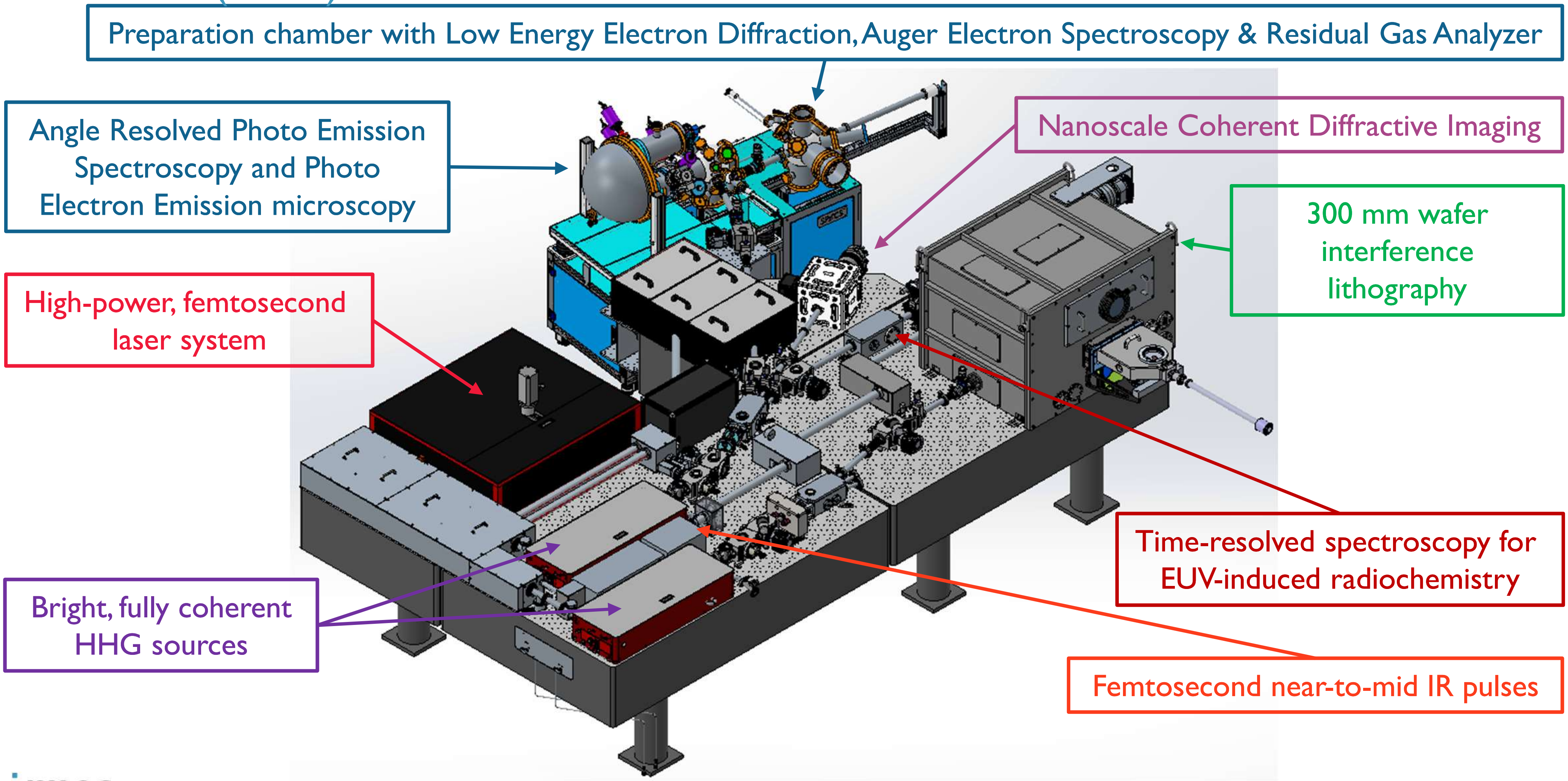
What next : 2D materials-Beyond CMOS

Photo Emission techniques

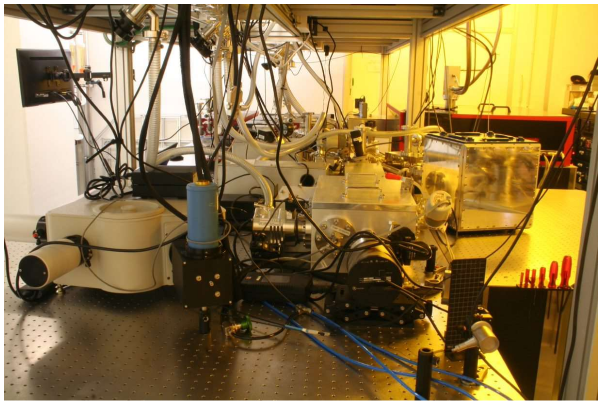
The imec AttoLab

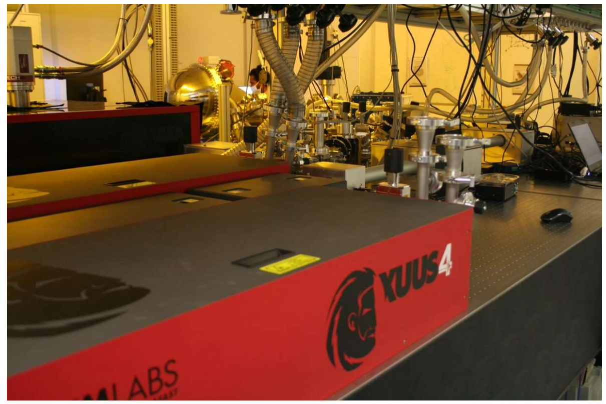
Results

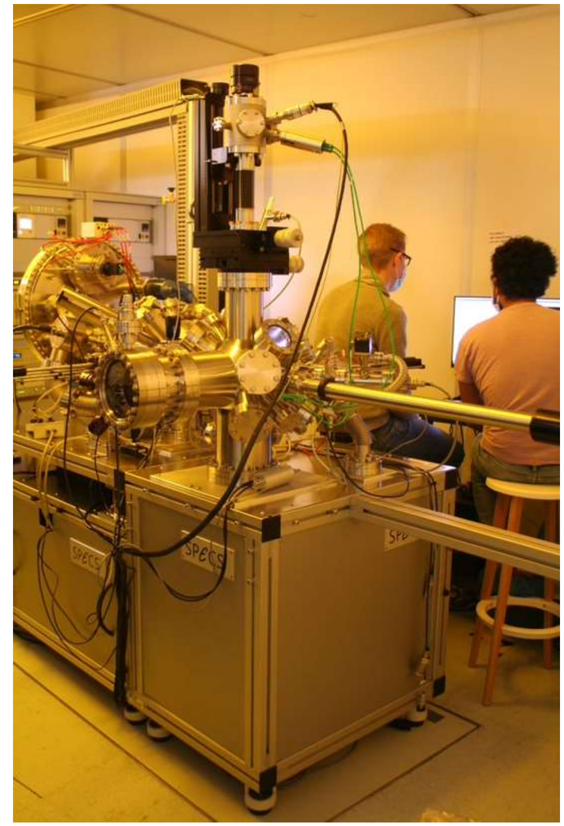
DESIGN (2019)

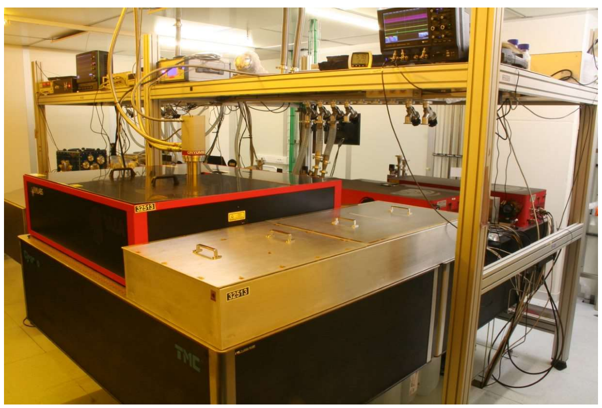

Preparation chamber with Low Energy Electron Diffraction, Auger Electron Spectroscopy & Residual Gas Analyzer
Angle Resolved Photo Emission Spectroscopy and Photo Electron Emission microscopy
Nanoscale Coherent Diffractive Imaging
300 mm wafer interference lithography
High-power, femtosecond laser system
Time-resolved spectroscopy for EUV-induced radiochemistry
Bright, fully coherent HHG sources
Femtosecond near-to-mid IR pulses

IT'S REAL (2020)









AGENDA

What next : 2D materials-Beyond CMOS

Photo Emission techniques

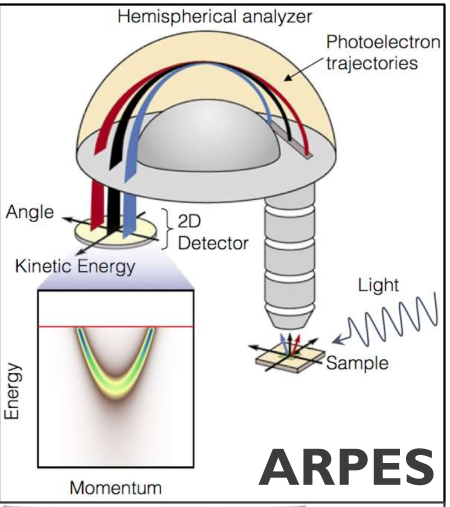
The imec AttoLab

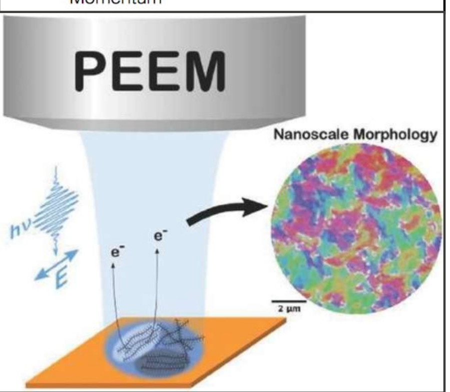
Results

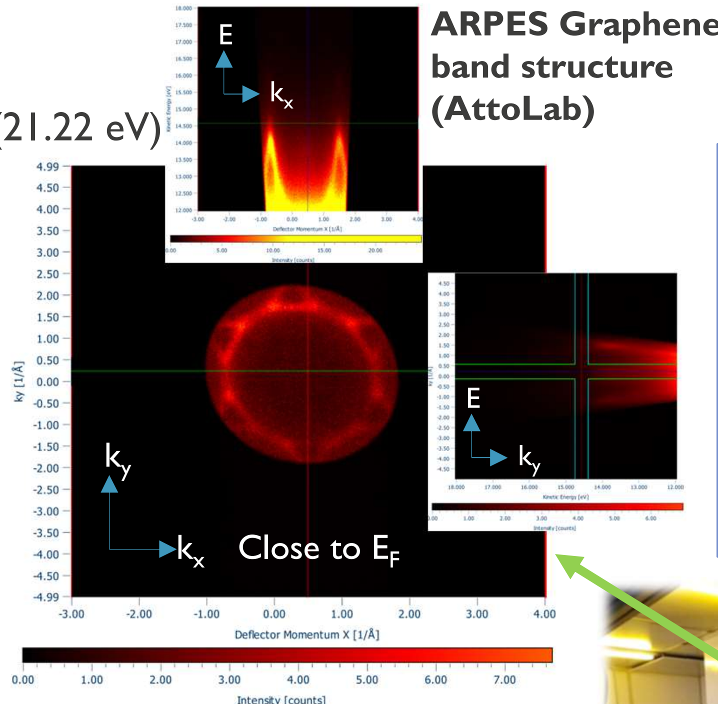
1ST RESULTS

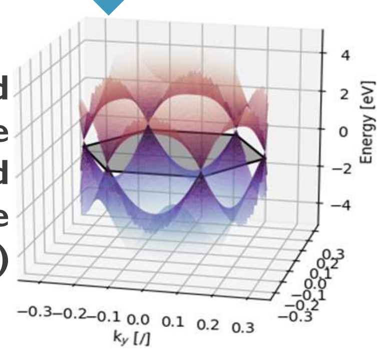
ARPES/PEEM with He I (21.22 eV)

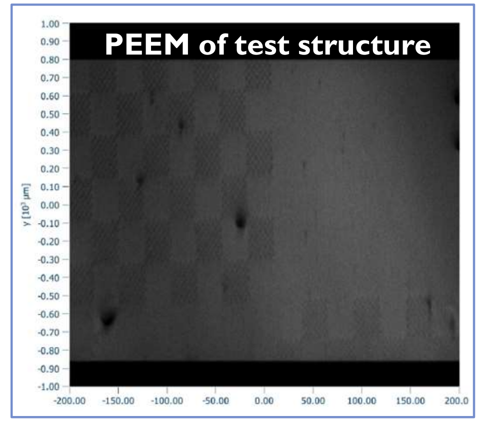
ARPES=Angle Resolved Photo Electron Spectroscopy
PEEM=Photo Electron Emission Microscopy
LEED=Low Energy Electron Diffraction
AES=Auge Electron Spectroscopy
L N_2=Liquid Nitrogen
L He=Liquid Helium

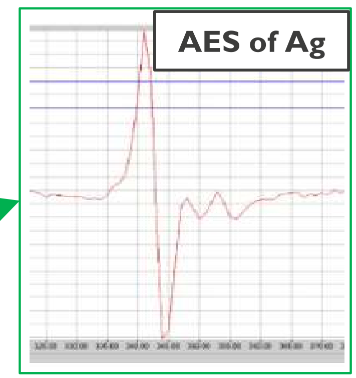


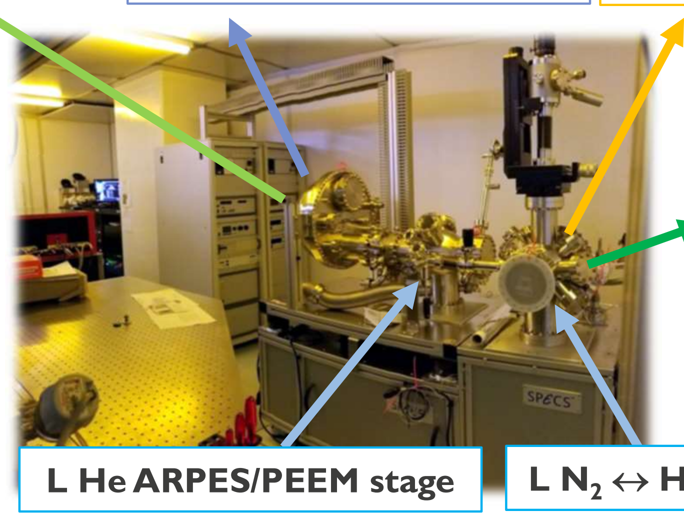










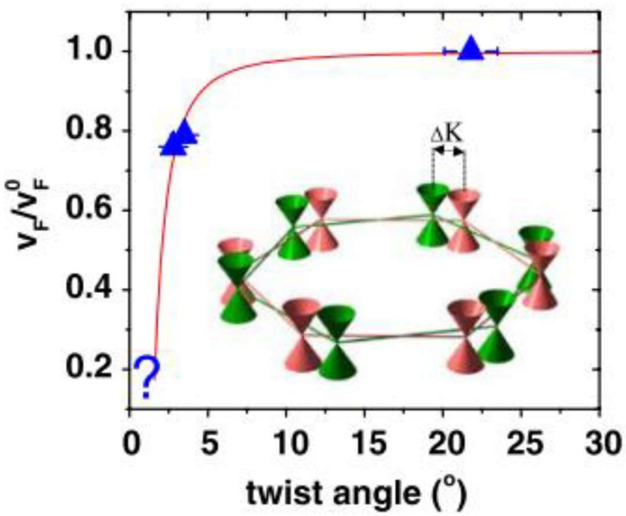


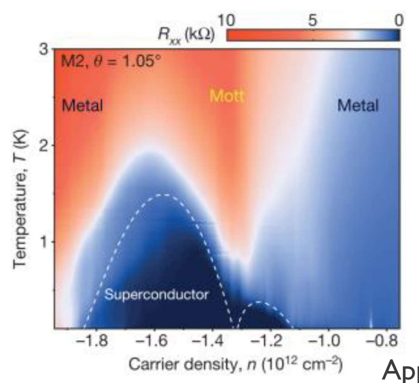
ARPES OF BI-LAYER GRAPHENE

ARPES/PEEM with He I (21.22 eV)

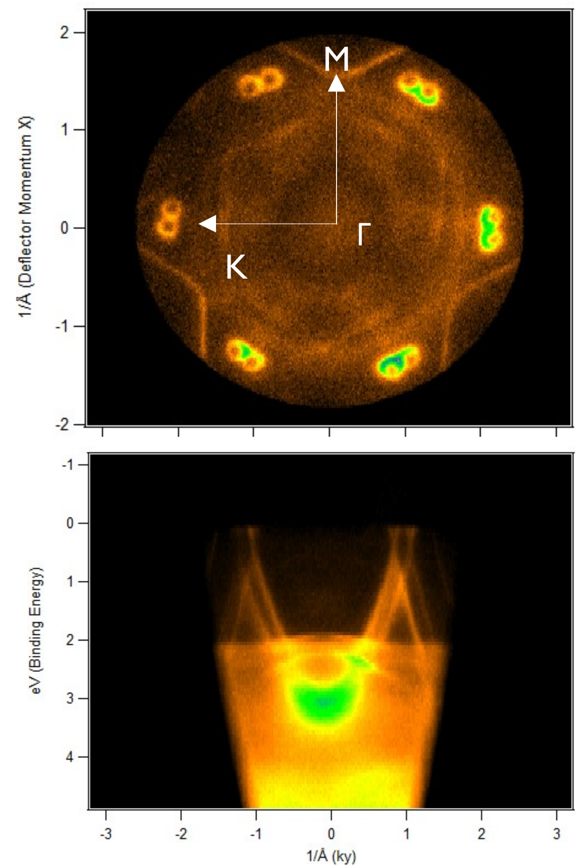
- ARPES of twisted bi-layer graphene show pairs of Dirac Cones
- This area of research is referred to as "twistronics"
- Why is this of interest:
  - When this equals 1.05° (termed the "magic angle" at which "van hove singularities" occur) superconductivity is noted (1st observed in 2018)

V^0_F = Fermi velocity in single layer graphene
V_F = Fermi velocity in bi-layer graphene





Twisted bi-layer

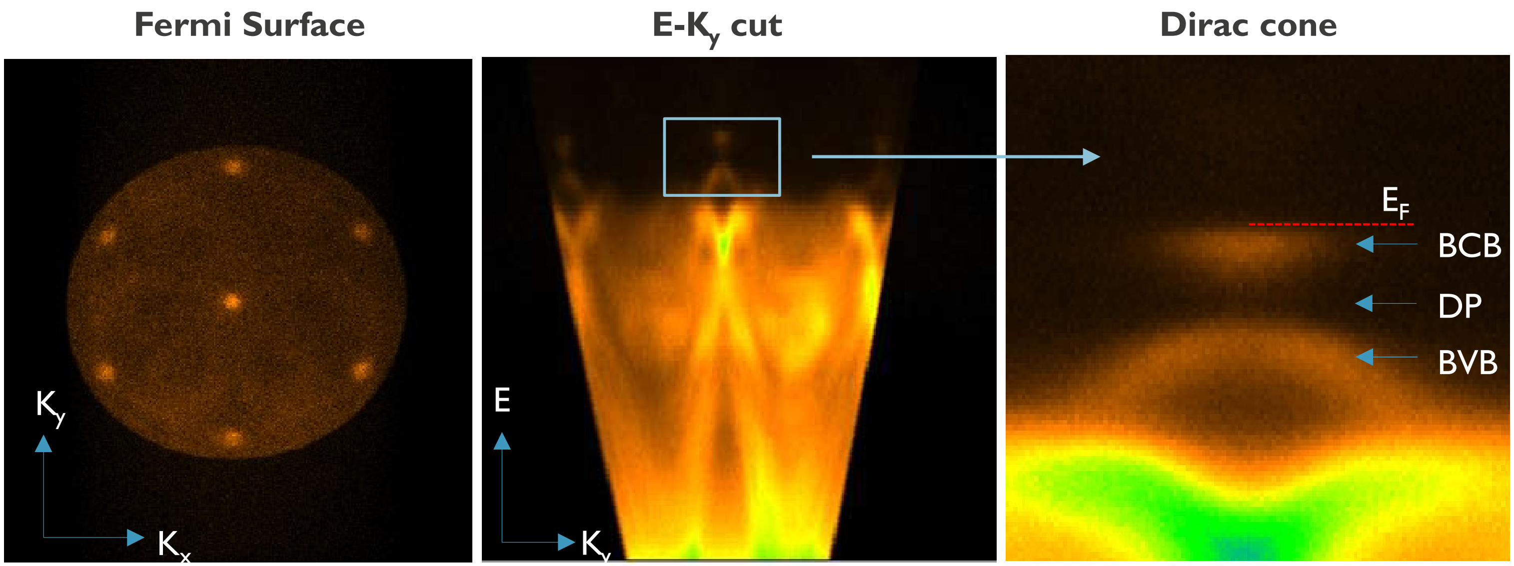


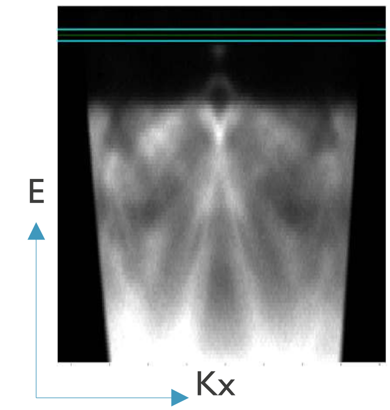
Appl. Sci. **2020**, 10, 4690; doi:10.3390/app10144690

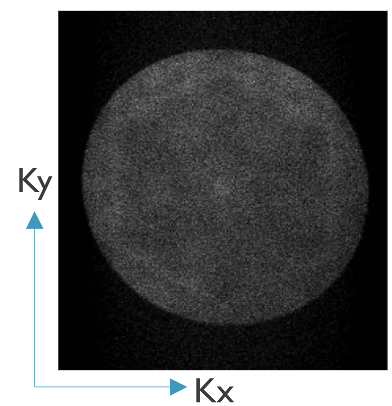
ARPES OF TOPOLOGICAL INSULATOR

ARPES/PEEM with He I (21.22 eV)

- Initial results from Bi_2Se_3
  - Note" since Bi_2Se_3 is air sensitive, this was capped with a thin film of Se which was subsequently burnt off within the ARPES prep chamber



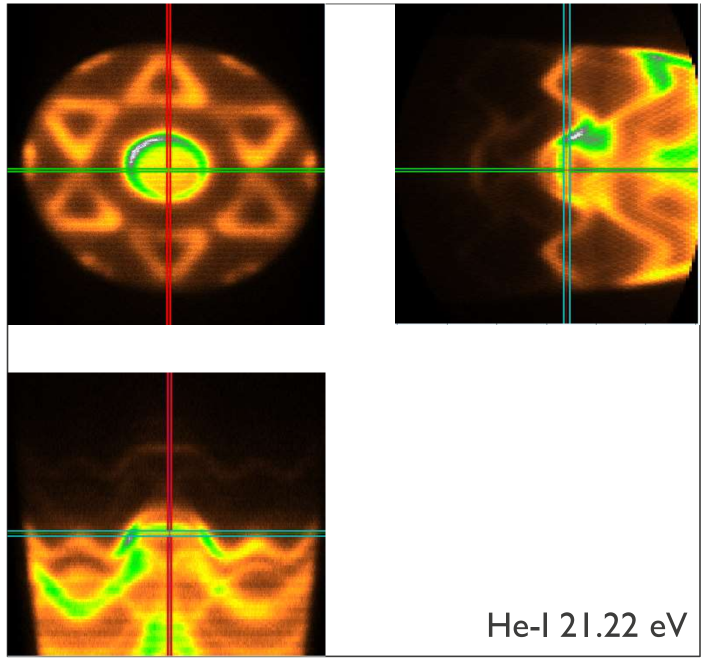


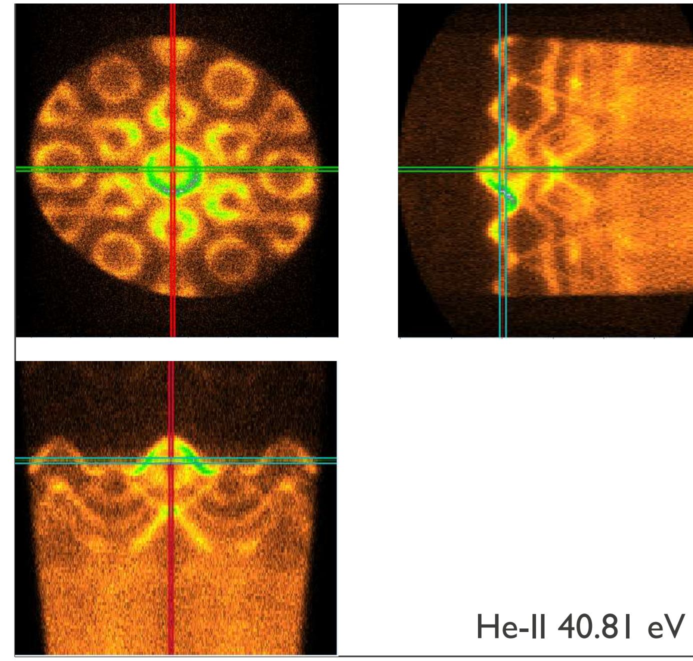


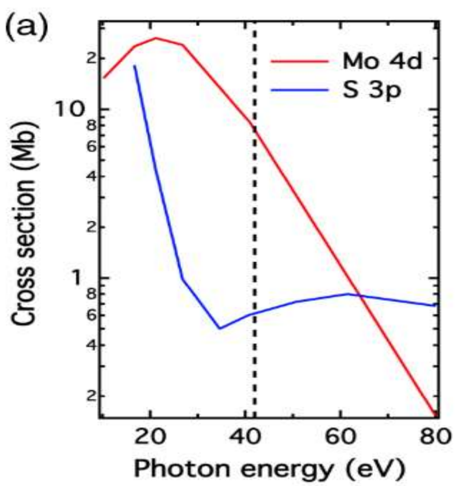
ARPES OF TMDs

ARPES with He I and He-II

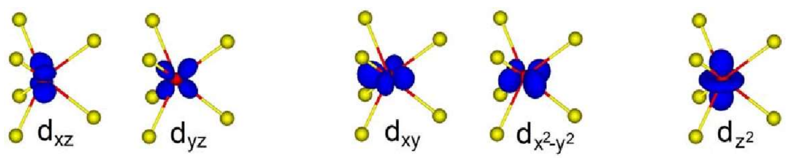
- ARPES of MoS_2 with He-I and He-II
- Different cross-sections

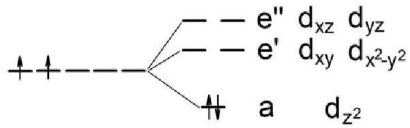


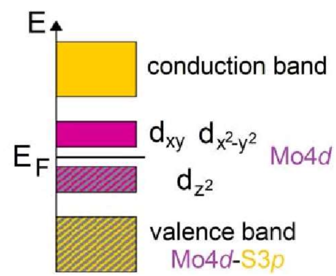




Jin et al., PRL 111, 106801 (2013)





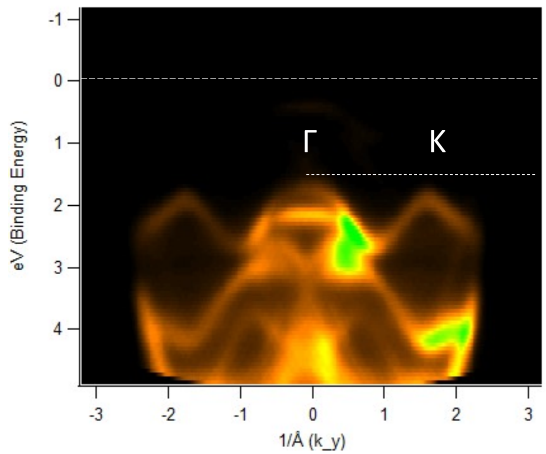


NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2014, 5 (4), P. 517–539

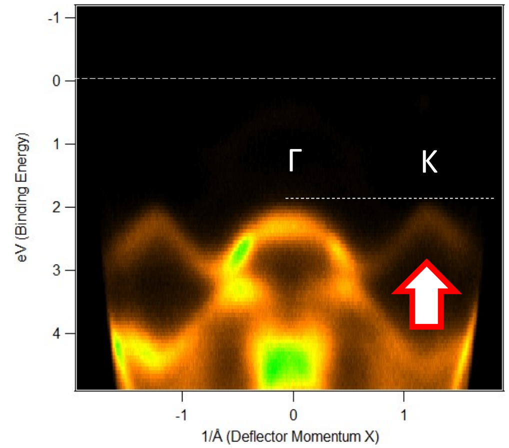
ARPES OF TMDs

ARPES/PEEM with He I

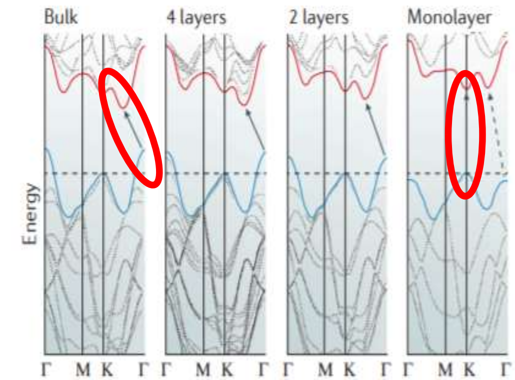
- Indirect to direct MoS_2 transition



3.5 ML

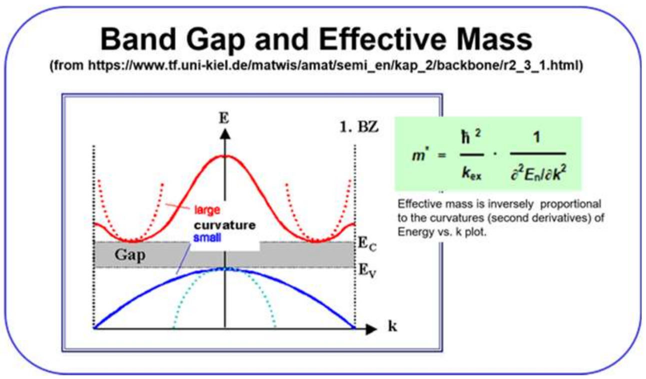


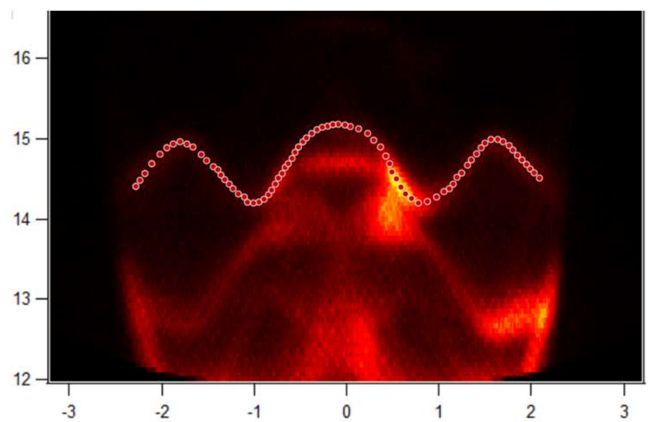
1 ML



Mazeli et al, Nature review Vol 2 | ARTICLE NUMBER 17033

- Derivation of electron mass (∝ 1/mobility)

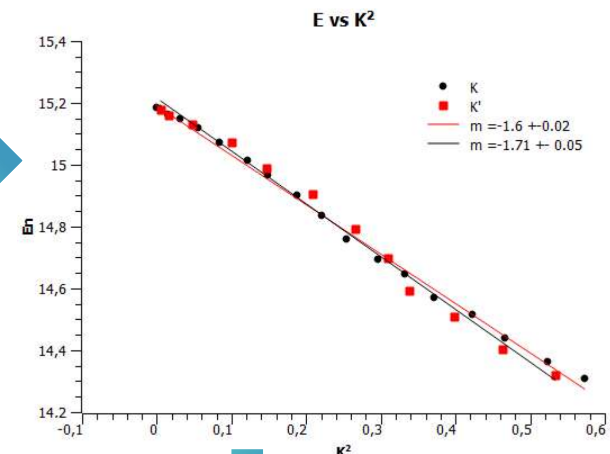




Literature: effective mass values

- Monolayer: (2.4 +- 0.3) m_o
- Bulk: (0.62 +- 0.01) m_o

DOI:10.1103/PhysRevLett.111.106801



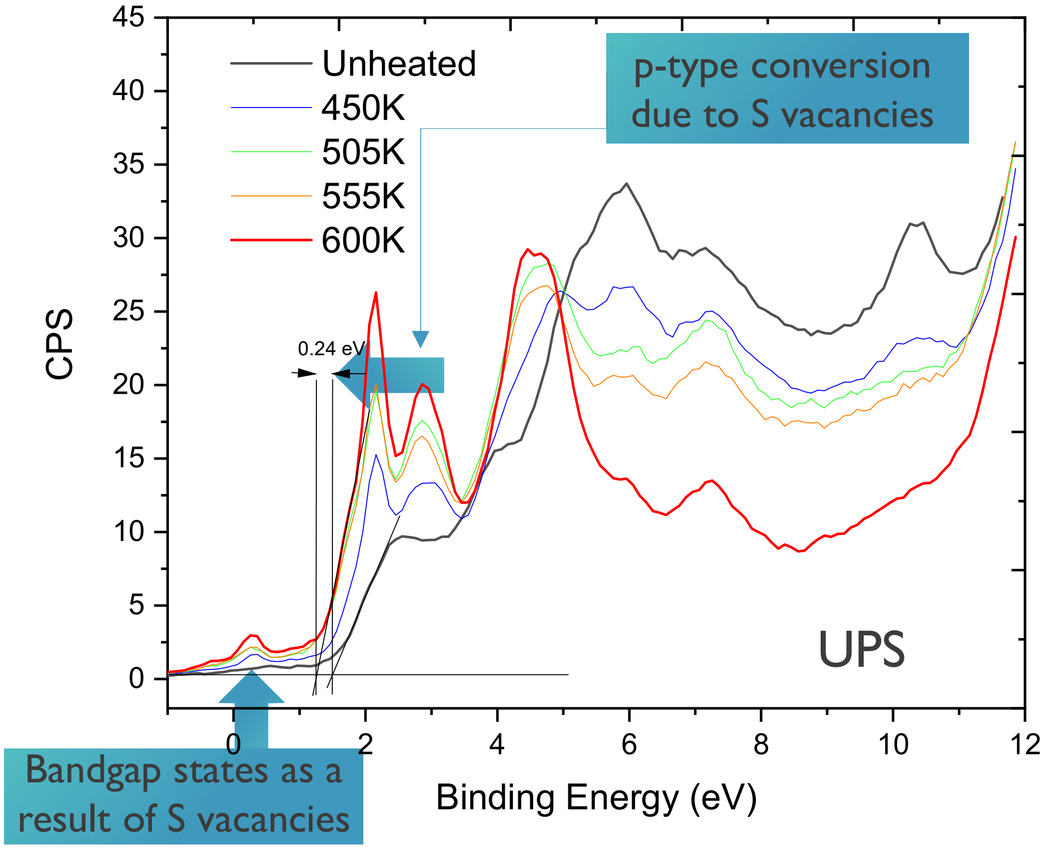
m= (2.3 ± 0.15) m_o

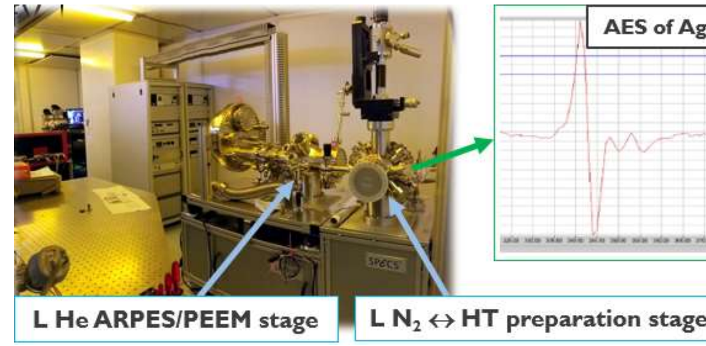
imec

PUBLIC

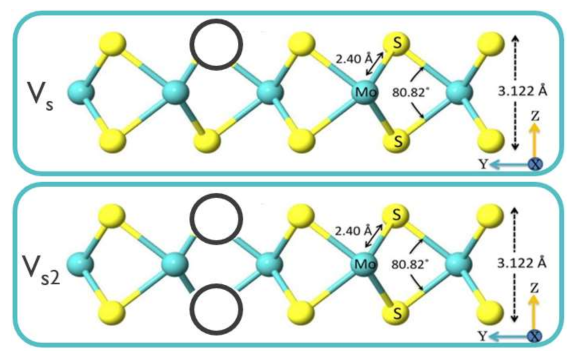
UPS of MoS_2: Annealing in-situ

UPS with He I (21.22 eV)





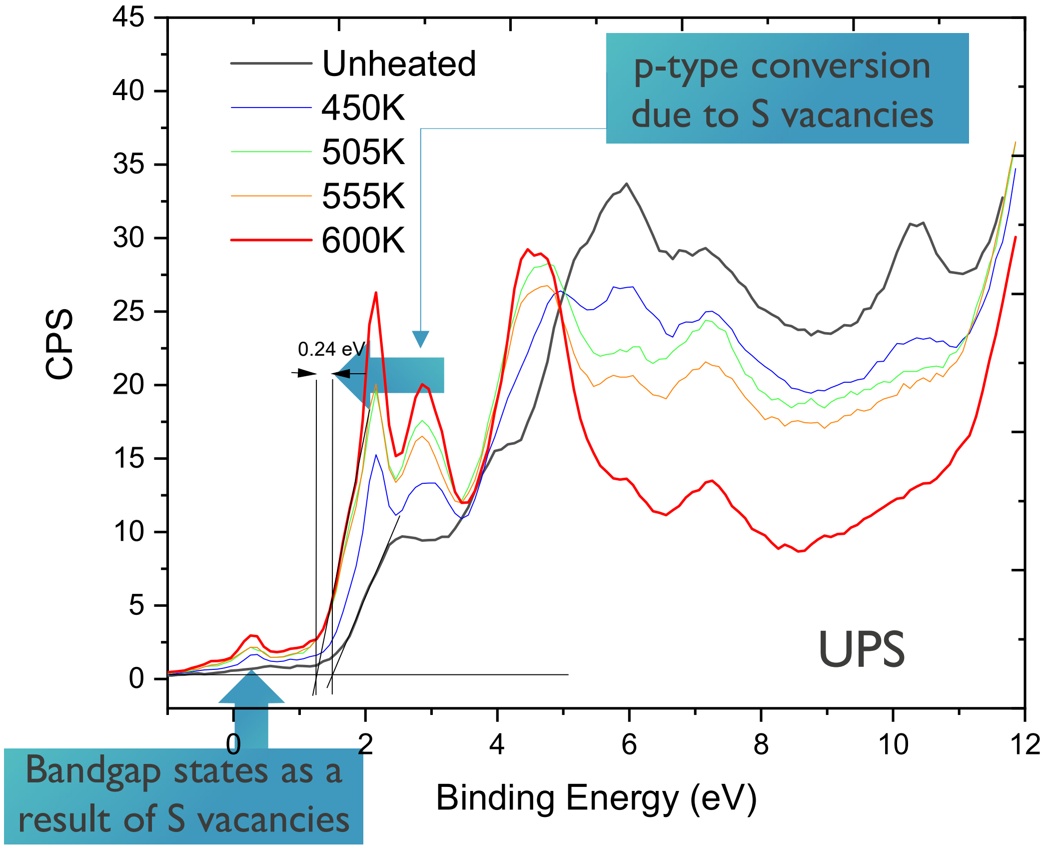
- UPS of MoS_2 before and after heating in prep chamber reveals
  - Conversion to p-type material (consistent with DFT simulations) due to S vacancies (V_S) generation

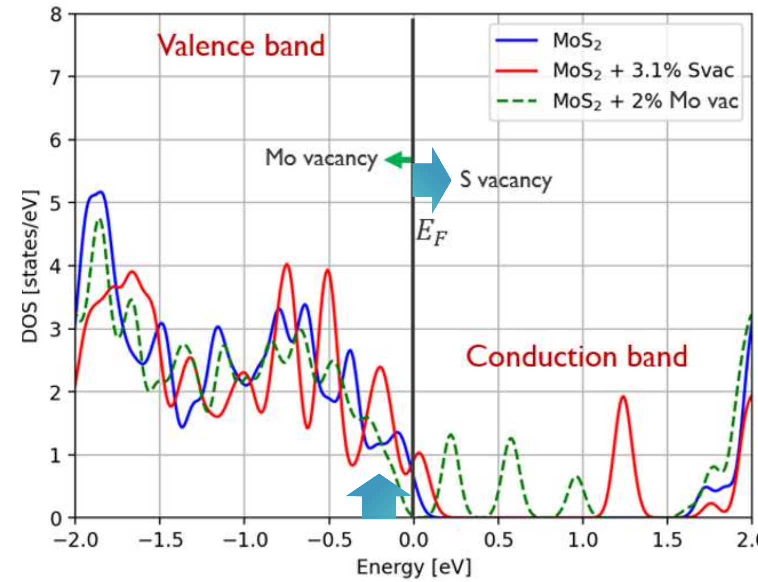


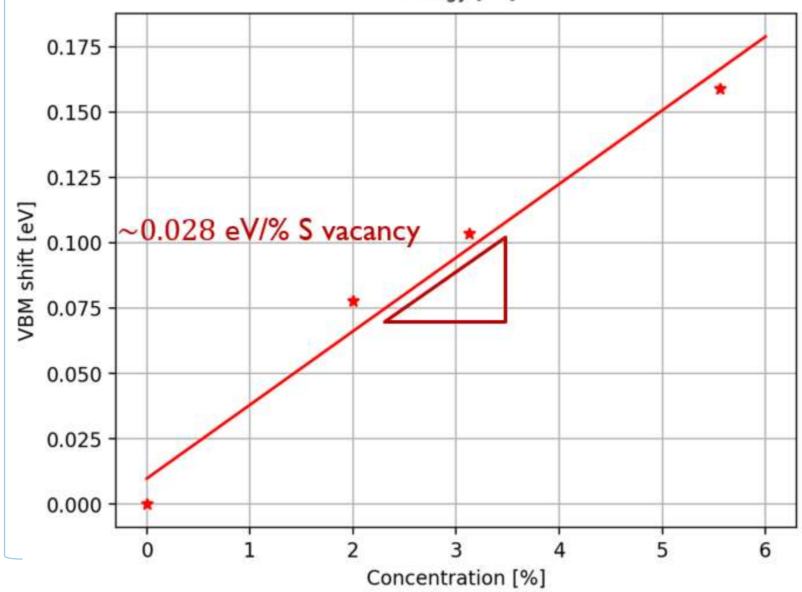
Cross-sectional views

UPS of MoS_2: Comparison with theory

DFT calculations care of MSP (imec)

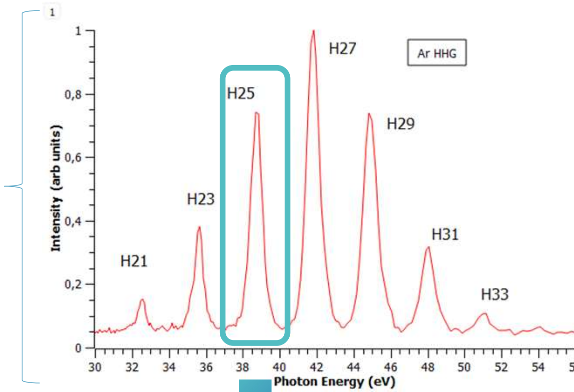


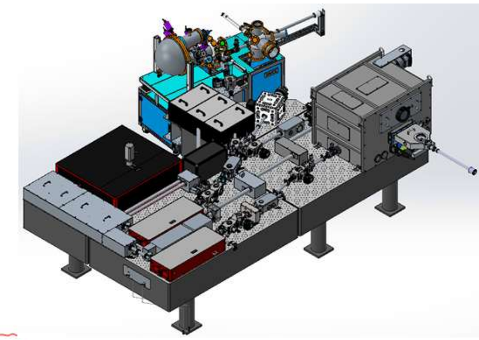




ARPES of MoS_2: 1st light

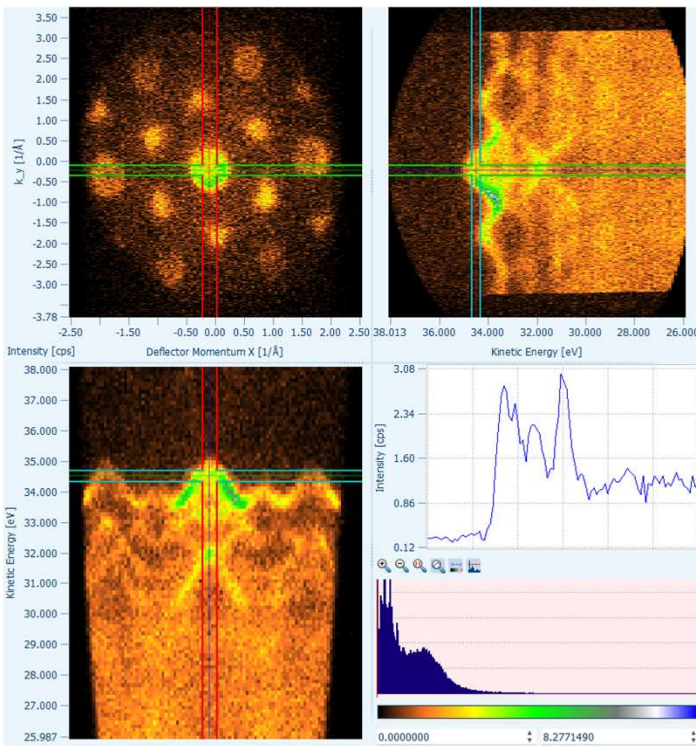
High Harmonic Generator source

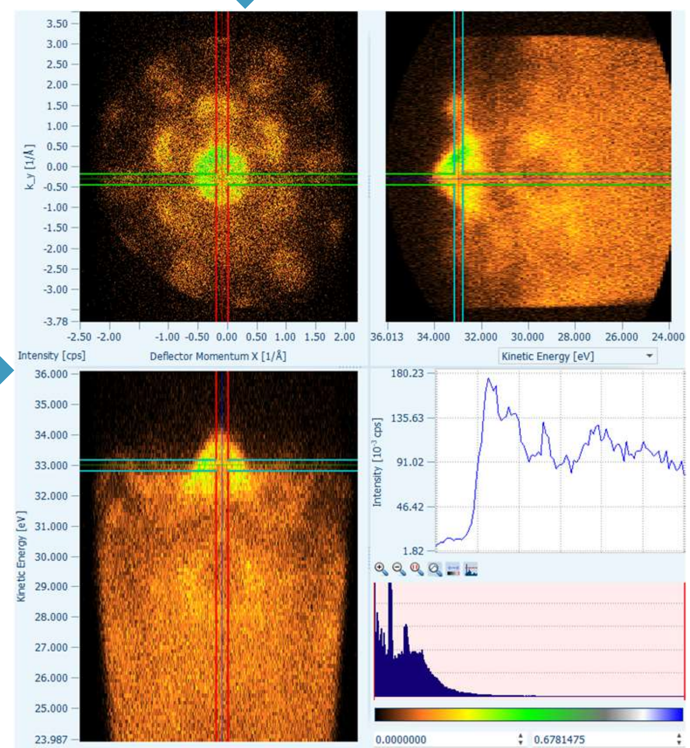




- First results from HHG source using 3rd harmonic compares well with He-II results

He-II (40.81eV)

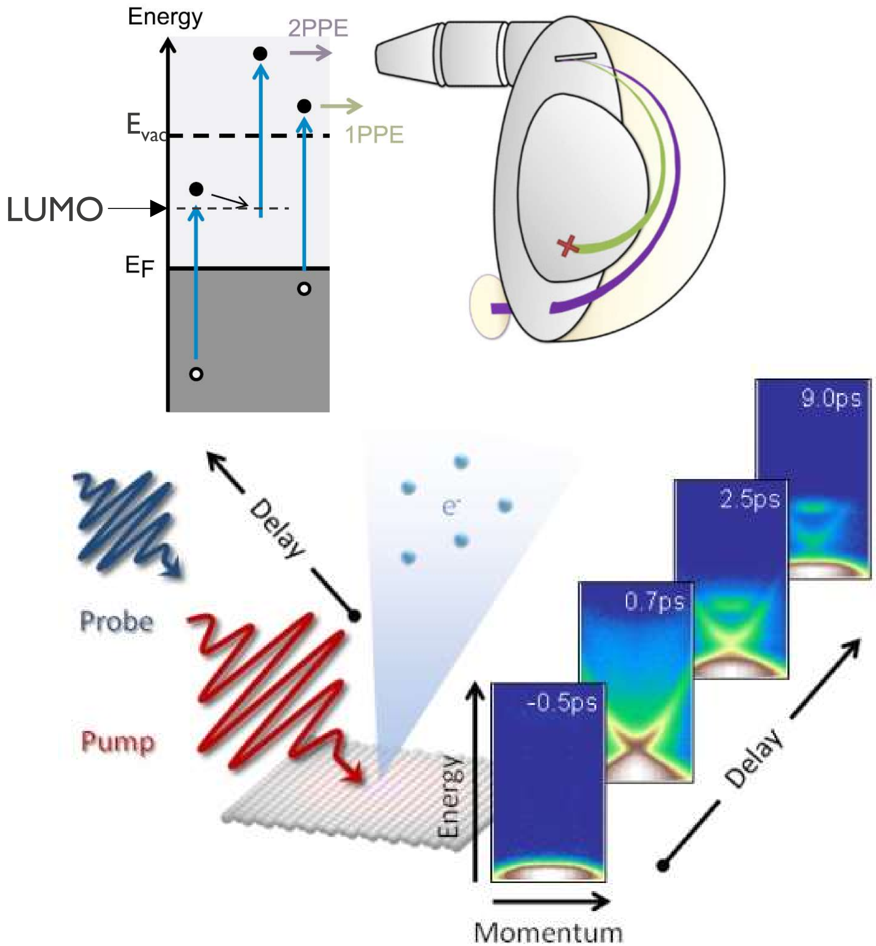


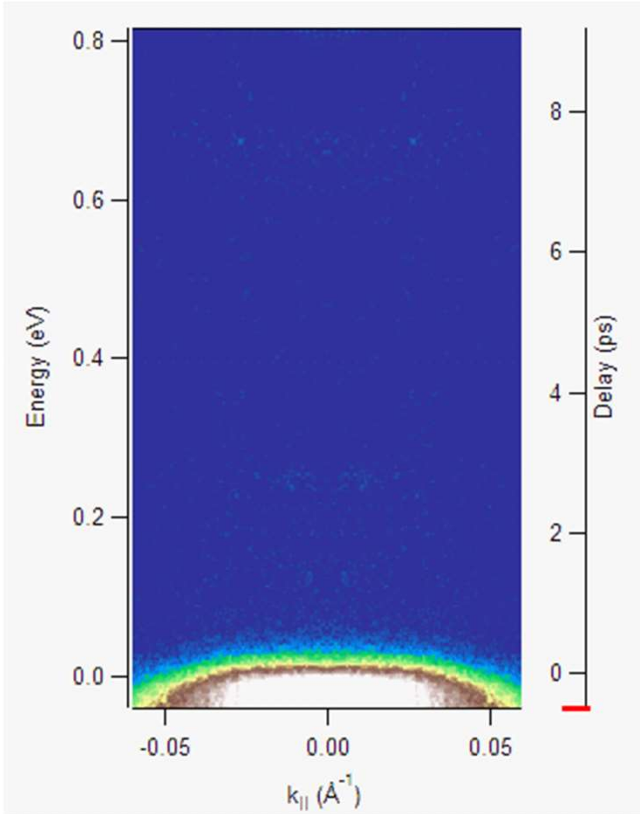


3rd HHG (39 eV)

WHAT NEXT?

- Pump-probe ARPES (2PPE) allows for states above E_F (LUMO) to be mapped
- Example from Bi_2Se_2 vs pump-probe delay time reveals kinetics





From: https://arpes.stanford.edu/research/tool-development/time-resolved-arpes#Approach

TIMELINES

- Implementation of AttoLab at imec
  - 2019: Design finalized, and funding realized
  - 2020: Laser bench and ARPES/PEEM/UPS with He source installed
  - 2020: 1st ARPES/PEEM/UPS results (from graphene followed by TI and TMDs)
  - 2021: Laser issues + Covid related supply chain issues
  - 2022: Al-kα source (1486.6 eV) installed allowing XPS
  - 2022: ARPES with laser (HHG source) realized

- Graphene, TMDs and TIs are 2D materials are crystalline materials that exhibit exotic properties of interest in beyond-CMOS device architectures.
- ARPES was the first technique to verify the existence of Topological Insulators (2007)
  - TIs were theoretically postulated in 2005 $\rightarrow$ 2016 Noble prize in physics

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The AttoLab team

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