Science Opportunities with Ultrahigh Resolution IXS Spectroscopy

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Outline

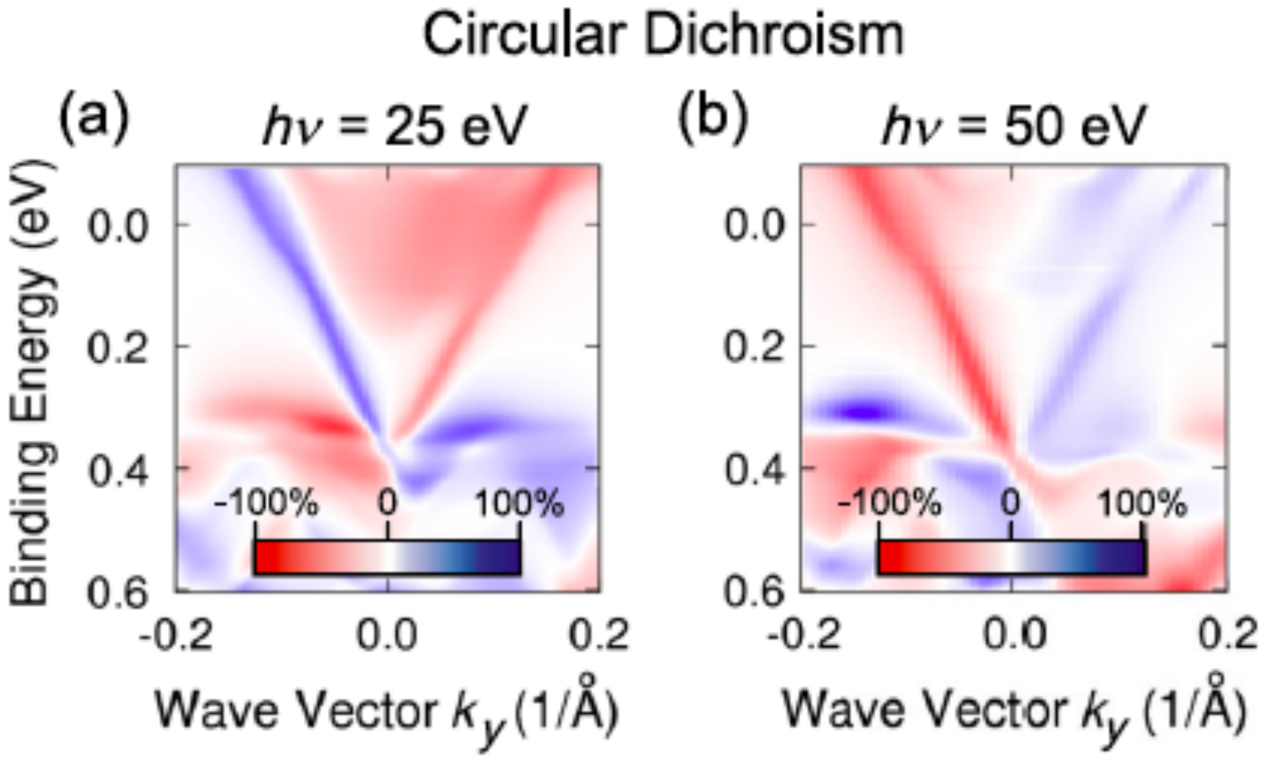
- Introduction and Overview
- Matrix Element Effect: ARPES / STM / RIXS
- Topological Physics at Low Energies
- Charge Response in Complex Materials
- Outlook and Conclusions

Introduction/Overview: $S(q,\omega)$

- Charge response; Picks up all charge excitations. $S(q,\omega) \sim$ (joint-density-of-states).
- No matrix element (challenge and opportunity); Intermediate states and core hole in RIXS.
- Truly bulk spectroscopy unlike ARPES and STM.
- Instrumental window of ~200 meV can capture much exciting physics of phonons and electrons, and through their couplings; Correlations / bonding effects extend to higher scales.

The Matrix Element Effect

ARPES and Spin Textures: Bi_2Te_3

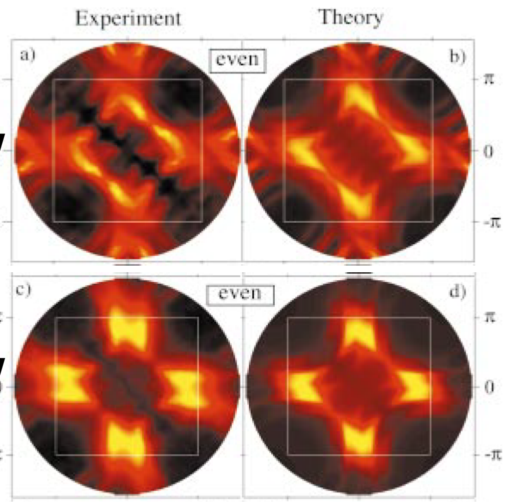


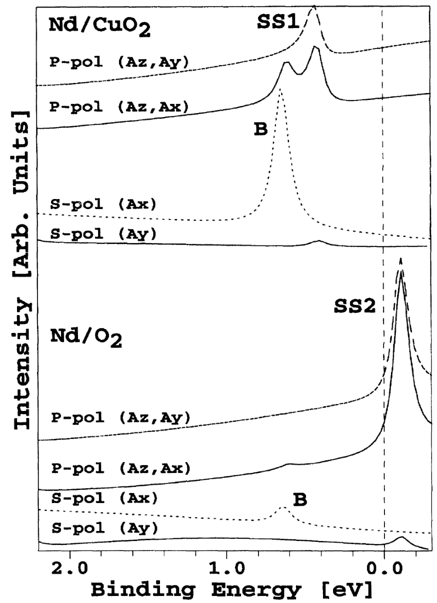
Scholz, Sanchez-Barriga, Braun, Marchenko, Varykhalov, Lindroos, Wang, Lin, Bansil, Minar, Ebert, Volykhov, Yashina, Rader, PRL (2013); Neupane et al., PRB 88, 165129 (2013).

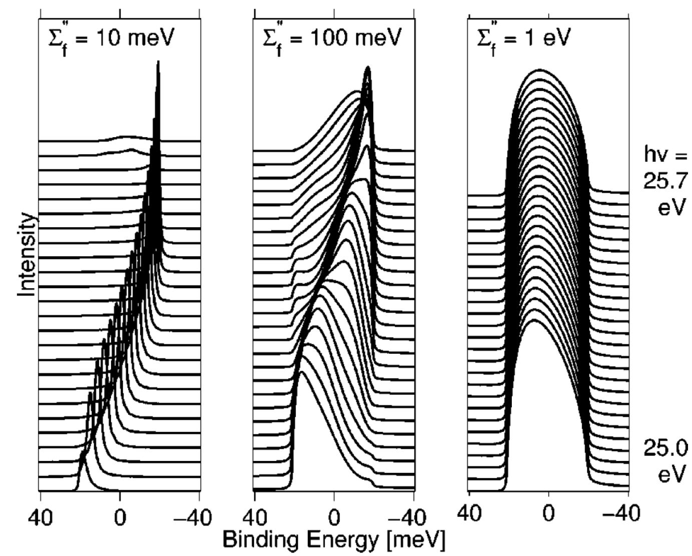
Nature of the ARPES Matrix Element

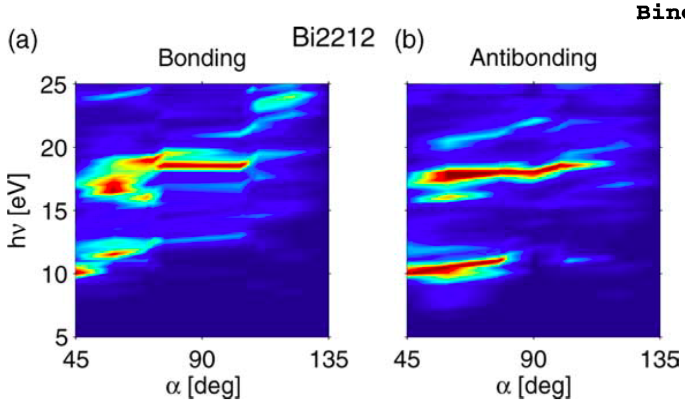
32 eV

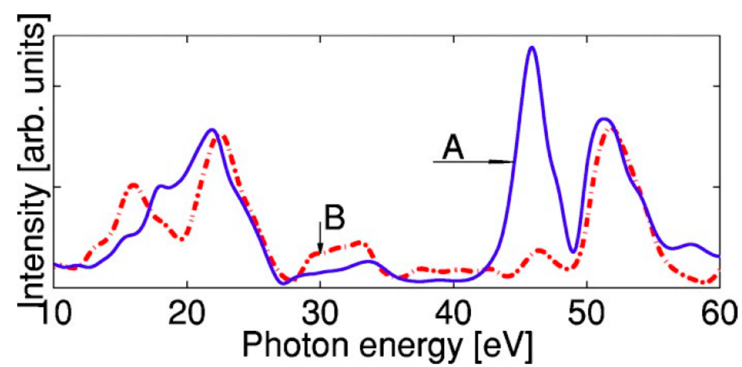
21 eV





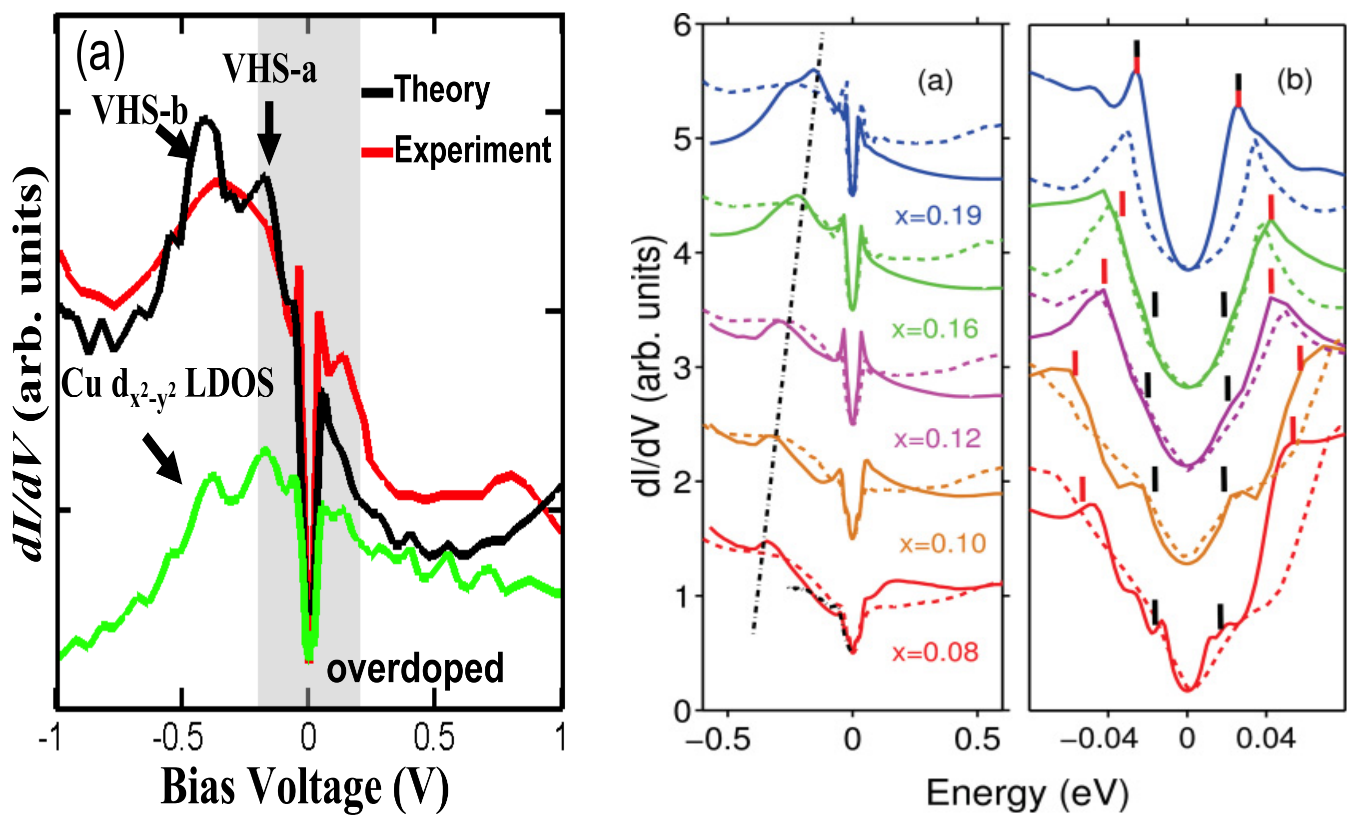






PRL (1995); PRB (2003); PRB (2004); PRL (2005); NJP (2005); JPCS (2006); JSNM (2012)

Bi2212: Asymmetries, Two-gap Physics, VHS

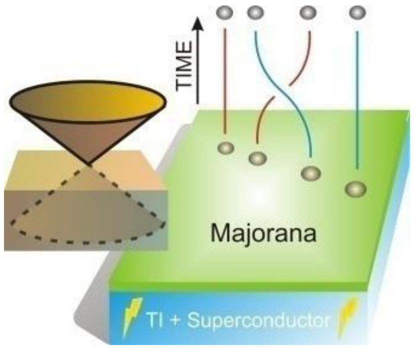


Theory: PRL102, 037001 (2009); PRB, 134509 (2009); PRB (2010); PRB (2011); PRB (2012)
Expt. (dashed): (a-right) McElroy et al., Science (2005); (b-right) Lawler et al., Nature (2010)

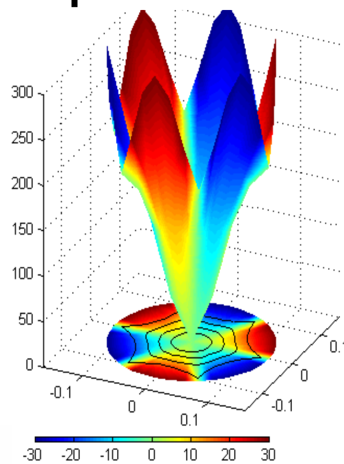
Topological Materials

- Quantum matter harbors many exotic phases beyond the topological insulators through the protections of time-reversal, crystalline and particle-hole symmetries.
- The band theory construct is continuing to provide a robust basis of predictive value for discovering new topological materials.
- Exotic fermions that have been the domain of high energy physics are becoming observable in desktop condensed matter systems.

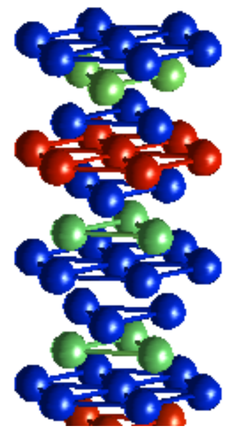
Predicting New Topological Insulators



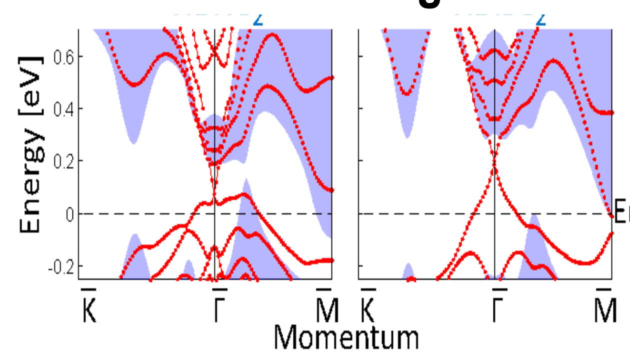
Spin texture

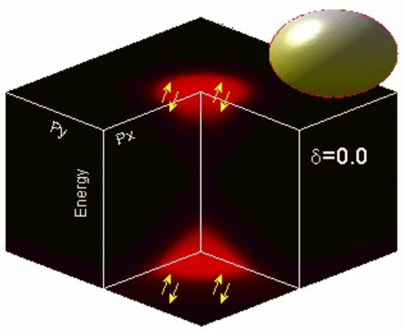


Germates

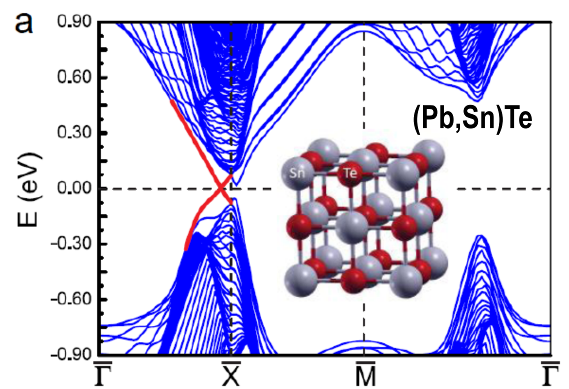


Tl-based chalcogenides



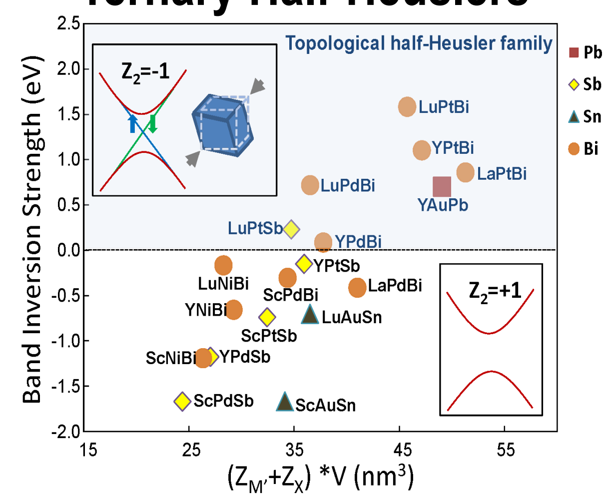


$TlBi(S_{1-\delta}Se_{\delta})_2$

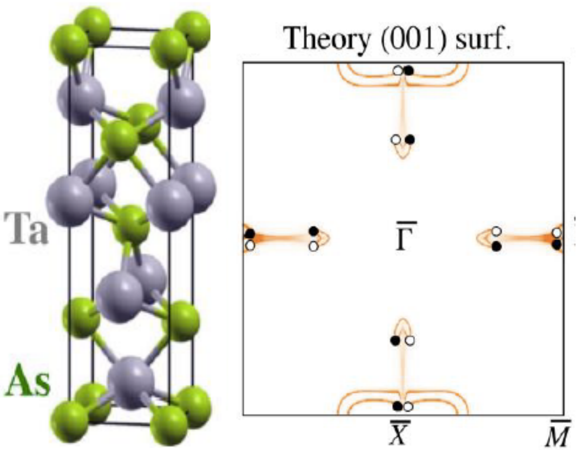


Topo. Crystalline Insulator

Ternary Half-Heuslers

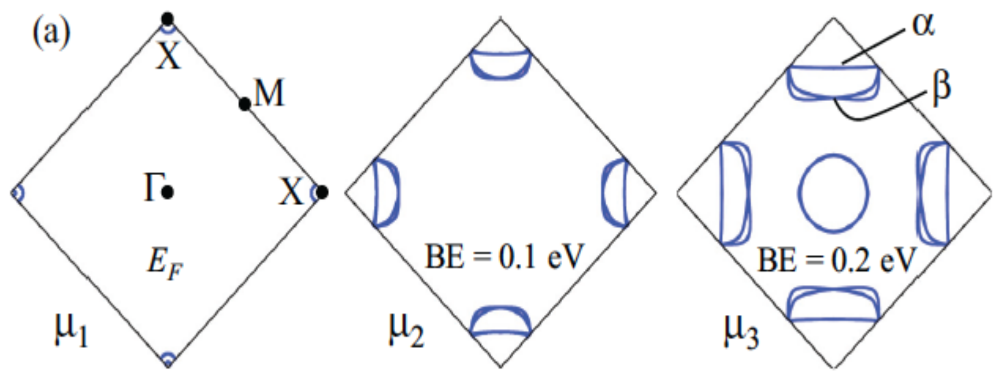


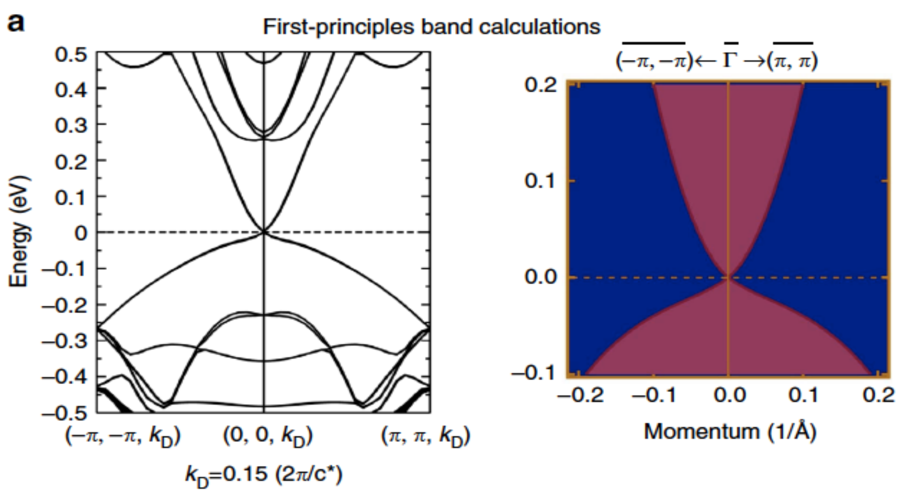
Predicting Other Topological Materials



Weyl semi-metal TaAs

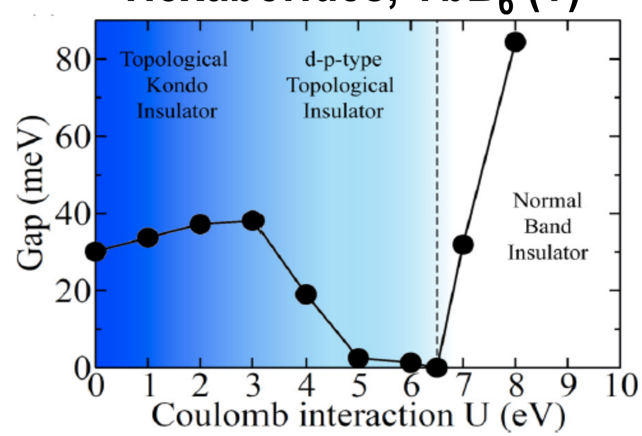
Iridates, Sr-327 (?)





Dirac fermions, Cd_3As_2; Na_3Bi

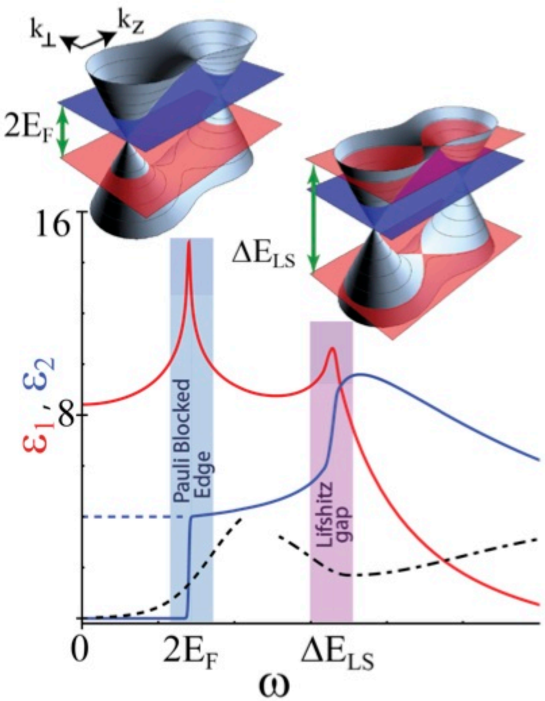
Hexaborides, YbB_6 (?)



Some Recent Work

- Science (2015); Nature Materials (2015a, 2015b); Science Advances (2015); Nature Physics (2015); Nature Commun. (2015a, 2015b, 2015c); PRL (2015a, 2015b, 2015c); Nano Letters (2015); ACS Nano (2015).
- Science Advances (2016); ACS Nano (2016); Nature Commun. (2016a, 2016b; 2016c); PNAS (2016); App. Phys. Lett. (2016a, 2016b); PRL (2016a, 2016b, 2016c).
- Bansil, Lin and Das: "Topological Band Theory," <u>Reviews of Modern Physics 88</u>, 021004 (2016).

Topological Physics at Low Energies



Dirac semi-metals: Na_3Bi and Cd_3As_2

- Optical signatures in JDOS from saddle points suppressed by selection rules due to s-orbital character of the Dirac bands. S(q,E) will see better.
- Rich structure of Dirac near Fermi energy should be accessible.
- Better phonon spectrum needed; optics suggests phase changes with temperature.

Jenkins, Lane, Barbiellini, Sushkov, Carey, Liu, Krizan, Kushwaha, Gibson, Chang, Jeng, Lin, Cava, Bansil, Drew et al. PRB B 94, 085121 (2016).

Topological Physics via IXS

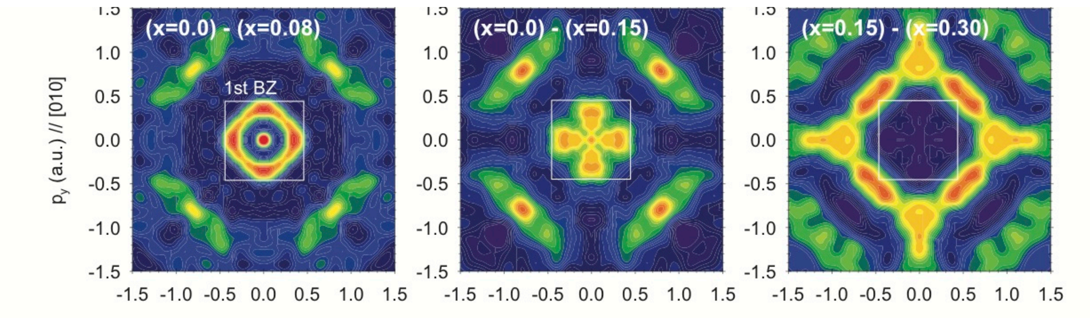
- Weyl semi-metals present even more complex FS topologies, should be accessible via IXS.
- Rich doping effects [Lifshitz transitions]; bulk to Dirac and Dirac to Dirac state transitions.
- Key surface state characteristics are controlled by bulk band topologies: opening of inverted gaps to identify topological phase transitions.
- Spectroscopy of topological band inversions and superconductivity under high pressures.
- Topological and others phases of ultrathin films (smaller volume advantage of proposed beamline)

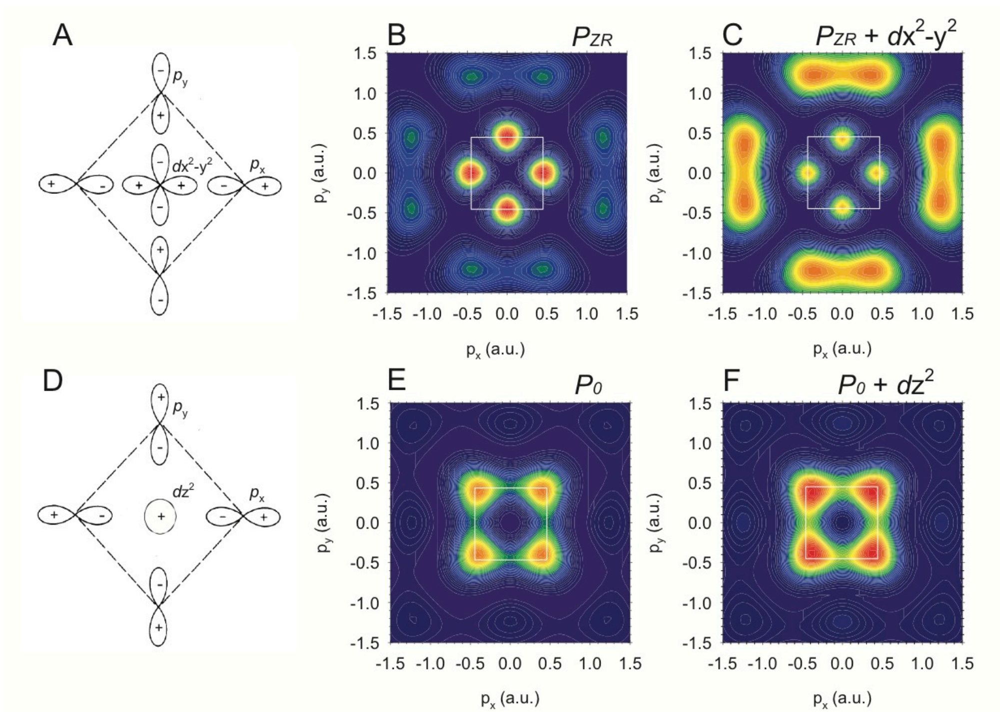
$S(q,\omega)$ in Higher BZ's

- $S(q,\omega)$ in higher zones codes details of electron-hole wave function at shorter distances. 1st BZ mainly captures the binding energy.
- Symmetry of intensity pattern in higher zones codes symmetry of the excited state.
- New beamline could thus enable new insights into the nature these states, nematicity, etc.

Wang, Barbiellini, Lin, Das, Basak, Mijnarends, Kaprzyk, Markiewicz, Bansil, PRB 85, 224529 (2012).

Compton limit of S(q,ω): Doped holes in LSCO

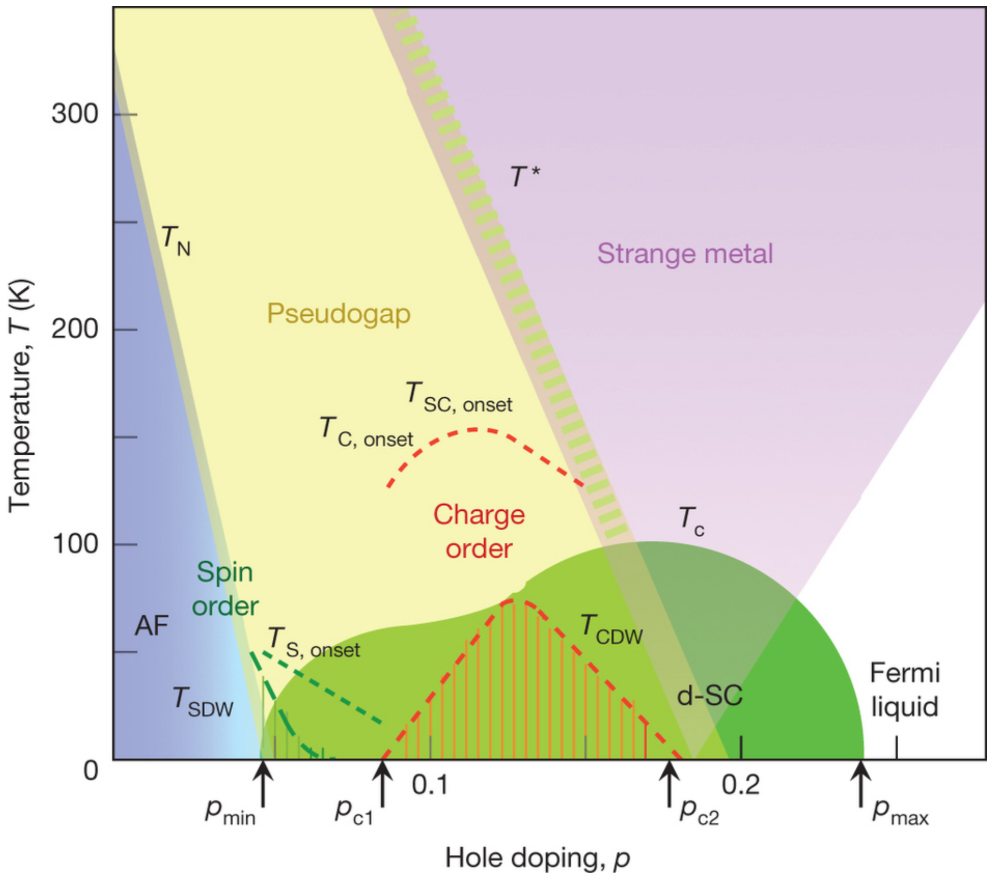




- Deeply inelastic scattering: Bulk sensitive (unlike ARPES, STS, transport), absolute spectral weights.
- Underdoped: Holes occupy Cu-d (x^2-y^2) & O-p(x,y) Zhang-Rice orbitals.
- Overdoped: d(x^2-y^2) & d(z^2) orbitals, two band picture.
- Establish high resolution Compton as a imaging tool.
- New possibilities with ultrahigh resolution.

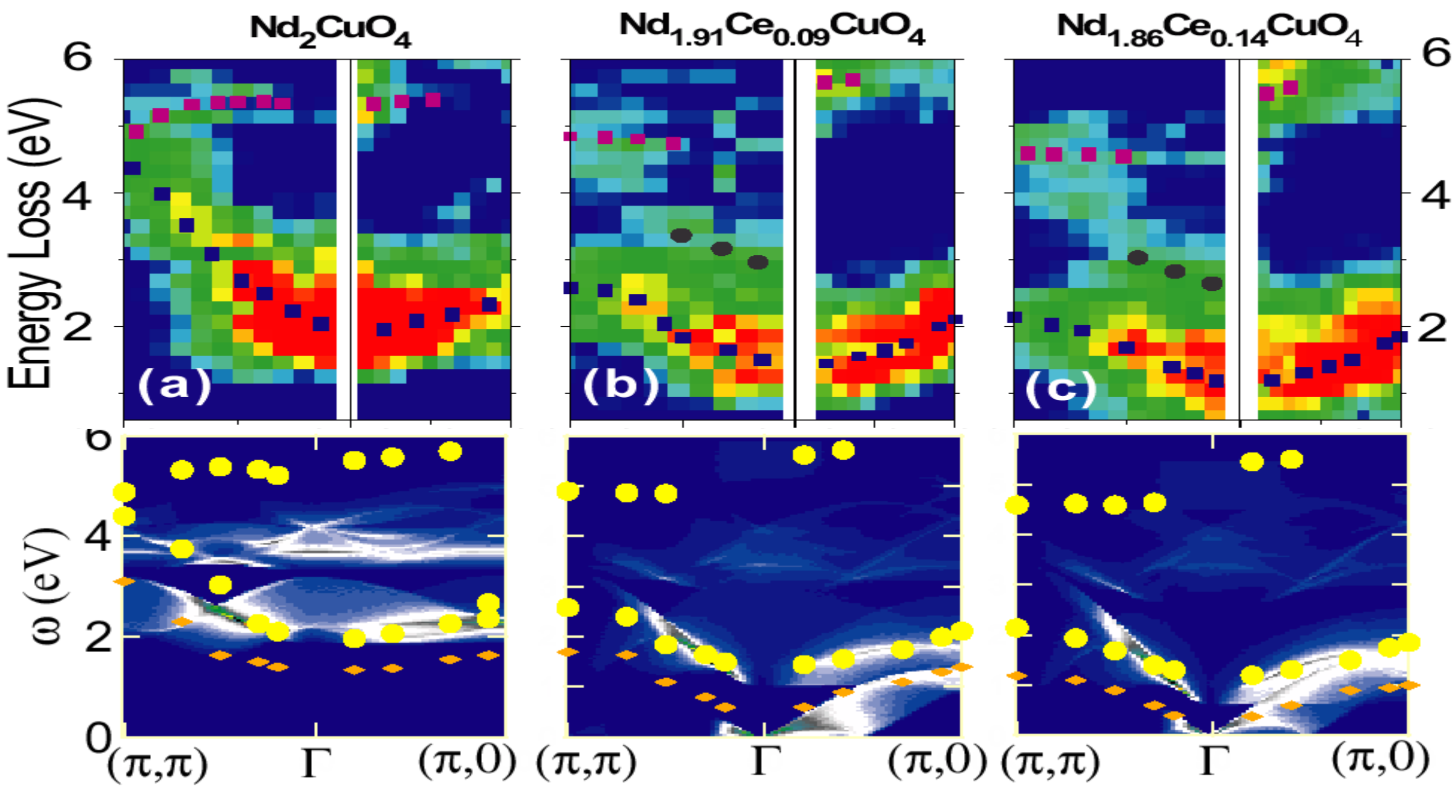
Sakurai, Itou, Barbiellini, Mijnarends, Markiewicz, Kaprzyk, Gillet, Wakimoto, Fujita, Basak Wang, Al-Sawai, Lin, Bansil, Yamada, Science 332, 698 (2011).

Charge Response in Complex Materials: Cuprates



- Spin sector mapped out; charge sector less so.
- Capture superconductivity, pseudogap physics, gap closings, soft phonons, nematicity.
- Rapid mapping with high throughput in current and future complex materials.

S(q,ω) at Higher ω: Gap Collapse in NCCO, RIXS



Markiewicz and Bansil, PRL 96, 107005 (2006); Susmita Basak, Tanmoy Das, Hsin Lin, M.Z. Hasan, R.S. Markiewicz, and A. Bansil, PRB 85, 075104 (2012).

Summary & Conclusions

- Proposed beamline will widely impact condensed matter physics, opening a new bulk-sensitive spectroscopic window on low energy physics.
- Discussed examples drawn from topological and correlation physics in materials.