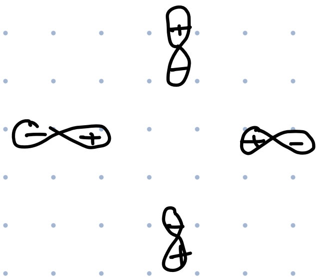
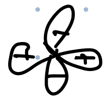
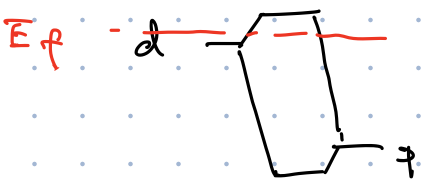
$\frac{1}{2}\Big($  $\Big)$ = "$L_{x^2-y^2}$"

 = $d_{x^2-y^2}$

$$\frac{1}{2}\times\left(\frac{\sqrt{3}}{2}\, pd\sigma \times 4\right) = \sqrt{3}\, pd\sigma$$

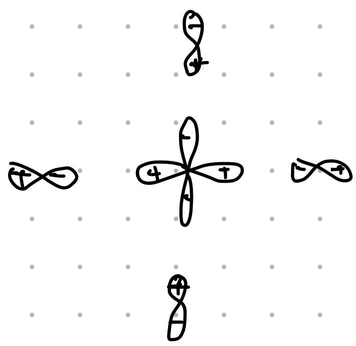
$$H_{dp^4} = \begin{pmatrix} \epsilon_d & \sqrt{3}\, pd\sigma \\ \sqrt{3}\, pd\sigma & \epsilon_L \end{pmatrix}$$



$$\frac{\epsilon_d + \epsilon_p}{2} \pm \sqrt{\left(\frac{\epsilon_d - \epsilon_p}{2}\right)^2 + 3\, pd\sigma^2}$$

↓ doping

Zhang-Rice singlet. PRB $\underline{37}$. 3759 (1988)



doping: 1 hole on $d_{x^2-y^2}$

1 hole on Ligand.

forms a singlet hopping on the Cu AFM background

Low-energy model:

$$H = \sum_{ij} t_{ij}\, c_i^\dagger c_j + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

single-band Hubbard model.

8.6. Dipole selection rules

How do we know that the low-energy model is correct? $\longrightarrow$ using spectroscopy.

In EM field. $\vec{p} \to \vec{p} - q\vec{A} = \vec{p} + e\vec{A}$. The light-matter interaction

$$H_{int} = H_{EM} - H_0 = \frac{(p+eA)^2}{2m} - \frac{p^2}{2m}$$

take the Coulomb gauge $\nabla \cdot A = 0$. then

$$H_{int} = \frac{e(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p})}{2m} + \frac{(eA)^2}{2m}$$

$$= \frac{e}{m}\vec{p}\cdot\vec{A}$$

non-linear term.

small for small $\vec{A}$.

$$\vec{A}(\vec{r}_i) = \frac{1}{\sqrt{V}} \sum_{k,\vec{\epsilon}} \sqrt{\frac{\hbar}{2\xi\omega}} \left(\vec{\epsilon}\, a_{\vec{k}\vec{\epsilon}}\, e^{i\vec{k}\cdot\vec{r}_i} + h.c. \right)$$

light polarization

Cross section for light absorption. $\mathcal{H} = \mathcal{H}_e \otimes \mathcal{H}_{ph}$.

$$\Omega = \frac{2\pi}{\hbar} \sum |\langle f | H_{int} | i \rangle|^2 \, \delta(E_f - E_i - \omega)$$

$$\langle f | H_{int} | i \rangle \propto e^{ikr} \langle f | \vec{\epsilon}\cdot\vec{p} | i \rangle$$

<u>core electrons.</u> $\propto e^{ikR} \langle f | \vec{\epsilon}\cdot[H, \vec{x}] | i \rangle$

$e^{ikr} \to e^{ikR}$ $\quad = e^{ikR} \langle f | \vec{\epsilon}\cdot(H\vec{x} - \vec{x}H) | i \rangle$

elec. $\quad$ nucleon $\quad = e^{ikR} (E_f - E_i) \langle f | \vec{\epsilon}\cdot\vec{x} | i \rangle$

The dipole operators $D_i = \vec{\epsilon} \cdot \vec{x}_i$

selection rules: The position in 3D can be expanded by vector operators: $\vec{x} = x_1 \hat{e}_1 + x_2 \hat{e}_2 + x_3 \hat{e}_3$

we choose a different basis: $r_q = r\, C_q^{(1)}$ $\quad q = 0, \pm 1$

$$C_q^{(1)} = \sqrt{\frac{4\pi}{2k+1}}\, Y_k^q(\hat{r})$$

$$r_{\pm 1} = \mp (x \pm i y)/2 \qquad r_0 = z.$$

$$\langle f | H_{int} | i \rangle \longrightarrow \langle n' l' m' | r\, C_q^{(1)} | n l m \rangle$$

$$= P^{(1)}_{n'l'nl} \langle l' m' | C_q^{(1)} | l m \rangle$$

$$P^{(k)}_{n'l'nl} = \int_0^\infty dr\, r^{k+2} R_{n'l'}(r) R_{nl}(r)$$

Wigner - Eckart:

$$\langle l' m' | C_q^{(k)} | l m \rangle = \underline{(-1)^{l'-m'} \begin{pmatrix} l' & k & l \\ -m' & q & m \end{pmatrix}} \; \underline{\langle l' \| C^{(k)} \| l \rangle}$$

$$\langle l' \| C^{(k)} \| l \rangle = (-1)^{l'} \sqrt{(2l+1)(2l'+1)} \begin{pmatrix} l' & k & l \\ 0 & 0 & 0 \end{pmatrix}$$

Dipole selection rules?

$$\begin{pmatrix} l' & k & l \\ -m' & q & m \end{pmatrix} \begin{matrix} \leftarrow \Delta l \le k = 1 \\ \leftarrow \underline{\underline{\Delta m = m' - m = 0, \pm 1}} \end{matrix}$$

$q = \pm 1, 0.$

$\begin{pmatrix} l' & k & l \\ 0 & 0 & 0 \end{pmatrix}$ requires $\Delta l \neq 0$. $\Rightarrow \underline{\underline{\Delta l = \pm 1}}$

($\forall m = 0$. $l' + k + l = \text{even}$)

⇒ dipole transition selection rule:

$$\begin{cases} \Delta l = \pm 1 \\ \Delta m = 0, \pm 1 \end{cases}$$

To probe Cu-3d. one need p or f.

Cu: $2p \longrightarrow 3d$

$l=2 \quad m = \pm 2$

$$d_{x^2-y^2} = \frac{1}{\sqrt{2}}\left(Y_{2,2} + Y_{2,-2}\right)$$

$$A \cdot \begin{array}{c} \begin{matrix} d & & p \end{matrix} \\ \begin{pmatrix} l' & 1 & l=1 \\ -m' & q & m \end{pmatrix} \end{array} \neq 0$$

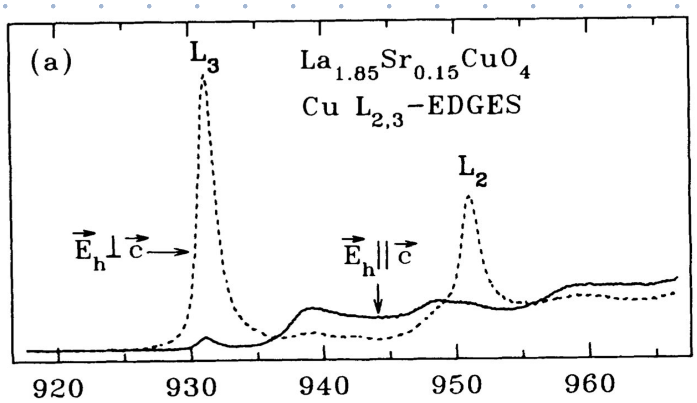
$m' = \pm 2 \quad |q| \leq 1 \quad \underline{\underline{|m| \leq 1}}$

$q = \pm 1 \quad m = 1$

$q = \pm 1$: $\vec{E}, \vec{r} \parallel x, y$ ✓

$\vec{E}, \vec{r} \parallel z, \quad m = 0$

$I_{XAS} \propto \langle \underline{n} \rangle$



From another view point:

$$\vec{r} \text{ behaves as } \left.\begin{array}{l} z \rightarrow A_{2u} \\ (x,y) \rightarrow E_u \end{array}\right\} \text{ in } D_{4h}.$$

(as well as p orb)

$$z \otimes p_z = A_{2u} \otimes A_{2u} = A_{1g}$$

$$z \otimes E_u = A_{2u} \otimes E_u = E_g$$

$$E_u \otimes A_{2u} = E_g$$

$$E_u \otimes E_u = A_{1g} \oplus A_{2g} \otimes \underline{\underline{B_{1g}}} \otimes B_{2g}$$

For optics. ($\sim$eV). transitions between valence states

$$\left.\begin{array}{l} A_{2g} \\ E_u \end{array}\right\} \otimes P = \underline{\qquad\qquad}.$$

$\uparrow$

dipole

9.7. superconducting order parameters

Ref: Annett. Advances in Physics. 39, 83 (1990)

Kaba & Sénéchal. PRB 100, 214507 (2019)

Use a simplified one-band model. (BCS equation)

$$H = \sum_{k\sigma} \epsilon_k c_{k\sigma}^+ c_{k\sigma} + \sum \underline{V_{kk'}} c_{k\uparrow}^+ c_{-k\downarrow}^+ c_{-k'\downarrow} c_{k'\uparrow}$$

electron-phonon coupling

AFM fluctuations etc.

It is sometimes possible to form "off-diagonal long-range order" (OLRO), or pairing

$$\Delta_k = -\sum_{k'} V_{kk'} \langle c_{-k'\downarrow} c_{k'\uparrow} \rangle$$

Mean-field decoupling : $cc \rightarrow \langle cc\rangle + (cc - \langle cc\rangle)$

$$H = \sum_{k\sigma} \epsilon_k c_{k\sigma}^+ c_{k\sigma} + \sum_{kk'} V_{kk'} c_{k\uparrow}^+ c_{-k\downarrow}^+ c_{-k'\downarrow} c_{k'\uparrow}$$

$$= \sum_{k\sigma} \epsilon_k c_{k\sigma}^+ c_{k\sigma} - \sum_k \left(\Delta_k c_{k,\uparrow}^+ c_{-k\downarrow}^+ + \bar{\Delta}_k c_{-k\downarrow} c_{k\uparrow}\right)$$

$$= \sum_k (c_{k\uparrow}^+ , c_{-k\downarrow}) \begin{pmatrix} \epsilon_k & \bar{\Delta}_k \\ \Delta_k & -\epsilon_{-k} \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow}^+ \end{pmatrix} + \text{const.}$$

diagonalized via a Bogoliubov transformation

$$\begin{pmatrix} \gamma_{k\uparrow} \\ \gamma_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} \bar{u}_k & v_k \\ -\bar{v}_k & u_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c^{+}_{-k\downarrow} \end{pmatrix}$$

$$\Rightarrow E_k = \sqrt{\epsilon_k^2 + |\Delta_k|^2}$$

We will not discuss more the superconductivity. but the form of Δ_k. In general. we can expand the order parameter as

$$\Delta_k = \sum_i c_i f^i(k)$$

(more generally. $\Delta_{k;mm';\sigma\sigma'} = \sum C_{\alpha\beta\gamma} f^{\alpha}(k) B^{\beta}_{mm'}(k) S^{\gamma}_{\sigma\sigma'}$ for multi-orbital case)

band spin

We are only discussing one-band singlet pairing.

How to expand? SC has a coherence length. (~ size of the Cooper pair). We can consider expansions on nearest neighbors.

$$f(k) \to \sum_r f_r \cdot e^{ikr}$$

The Fourier coefficient f_r decays over space.

Consider local pairing $\Delta_k = f_0$ A_{1g}

Consider nearest neighbors $\vec{r} = \hat{x}, \hat{y}$

The four basis function $(e^{ik_x}, e^{-ik_x}, e^{ik_y}, e^{-ik_y})$

Similar to the previous section, we can construct projectors and find eigenstates

$$P_{A_1} = \frac{1}{4}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} \qquad \psi = \frac{1}{2}(1, 1, 1, 1)^T$$

The A_1 symmetry is $\frac{1}{2}(e^{ik_x} + e^{ik_y} + e^{-ik_x} + e^{-ik_y})$

$= \cos k_x + \cos k_y$

eigenstates of P_{B_1}: $\frac{1}{2}(1, -1, 1, -1)^T$

B_1 symmetry: $\frac{1}{2}(\cos k_x - \cos k_y)$

See mathematica notebook for details.

2nd neighbor: $\{e^{i(k_x+k_y)}, e^{i(k_x-k_y)}, e^{-i(k_x+k_y)}, e^{-i(k_x-k_y)}\}$

$V \cong A_1 + B_2 + E$

$A_1 = 2\cos k_x \cos k_y$

$B_2 = 2\sin k_x \sin k_y$

E: $\sin(k_x + k_y)$

$\sin(k_x - k_y)$

3rd neighbor the same as 1st.

4th neighbor. 8-dim rep. space.

E pairing is odd in space → triplet pairing

also → $\sin k_x \pm i \sin k_y$ related by time reversal

gap measurements

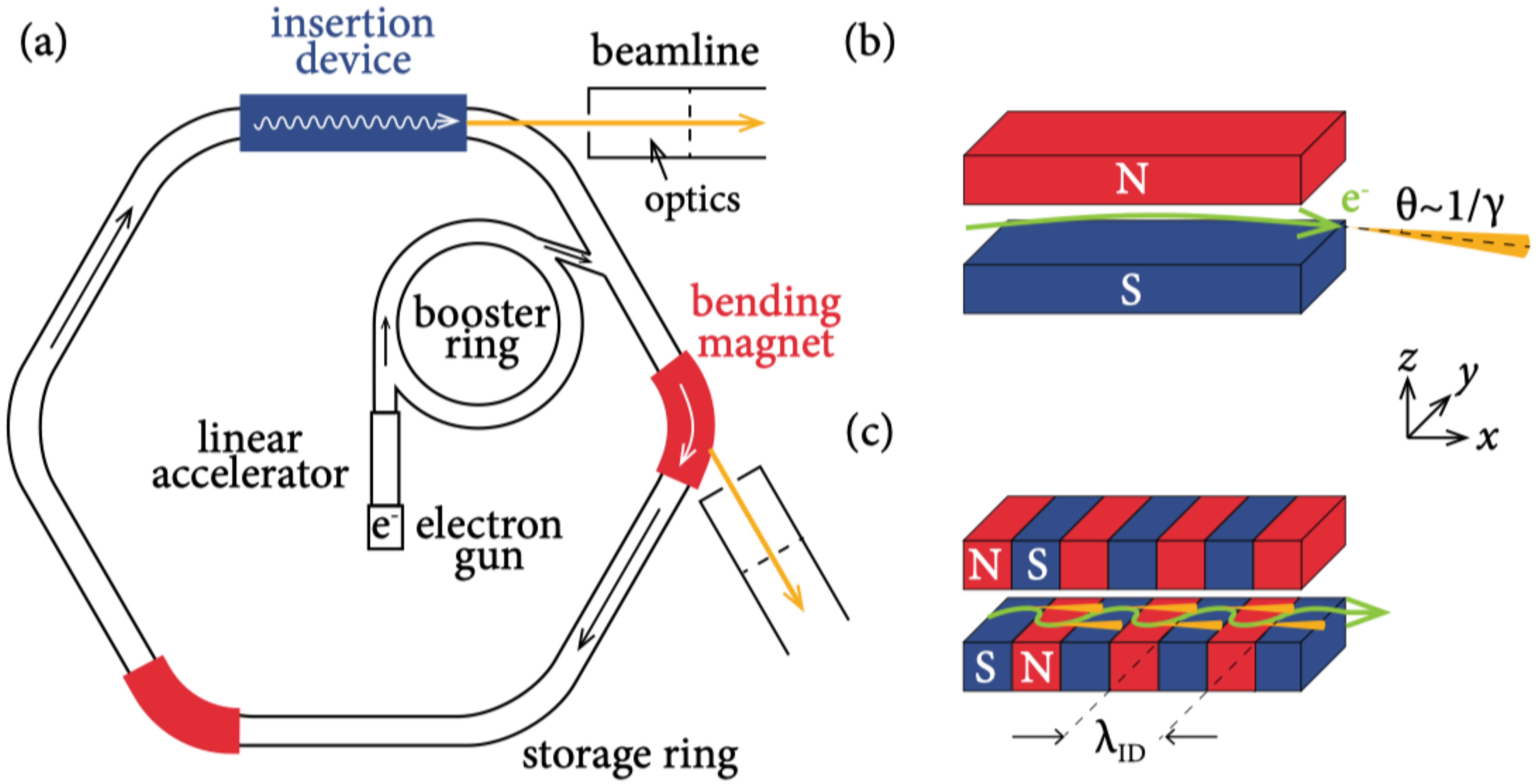
- transport
- ARPES

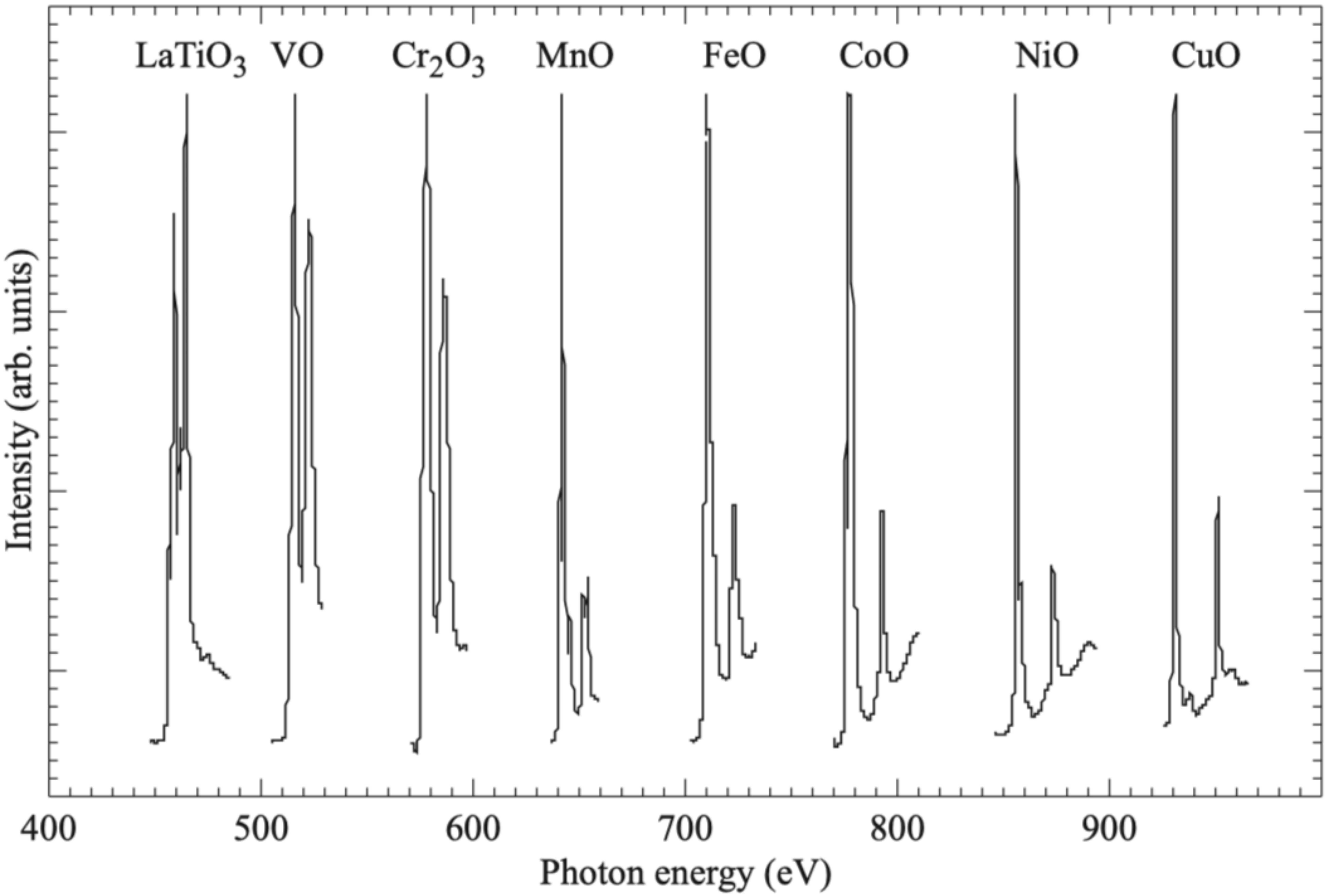
Josephson tunneling

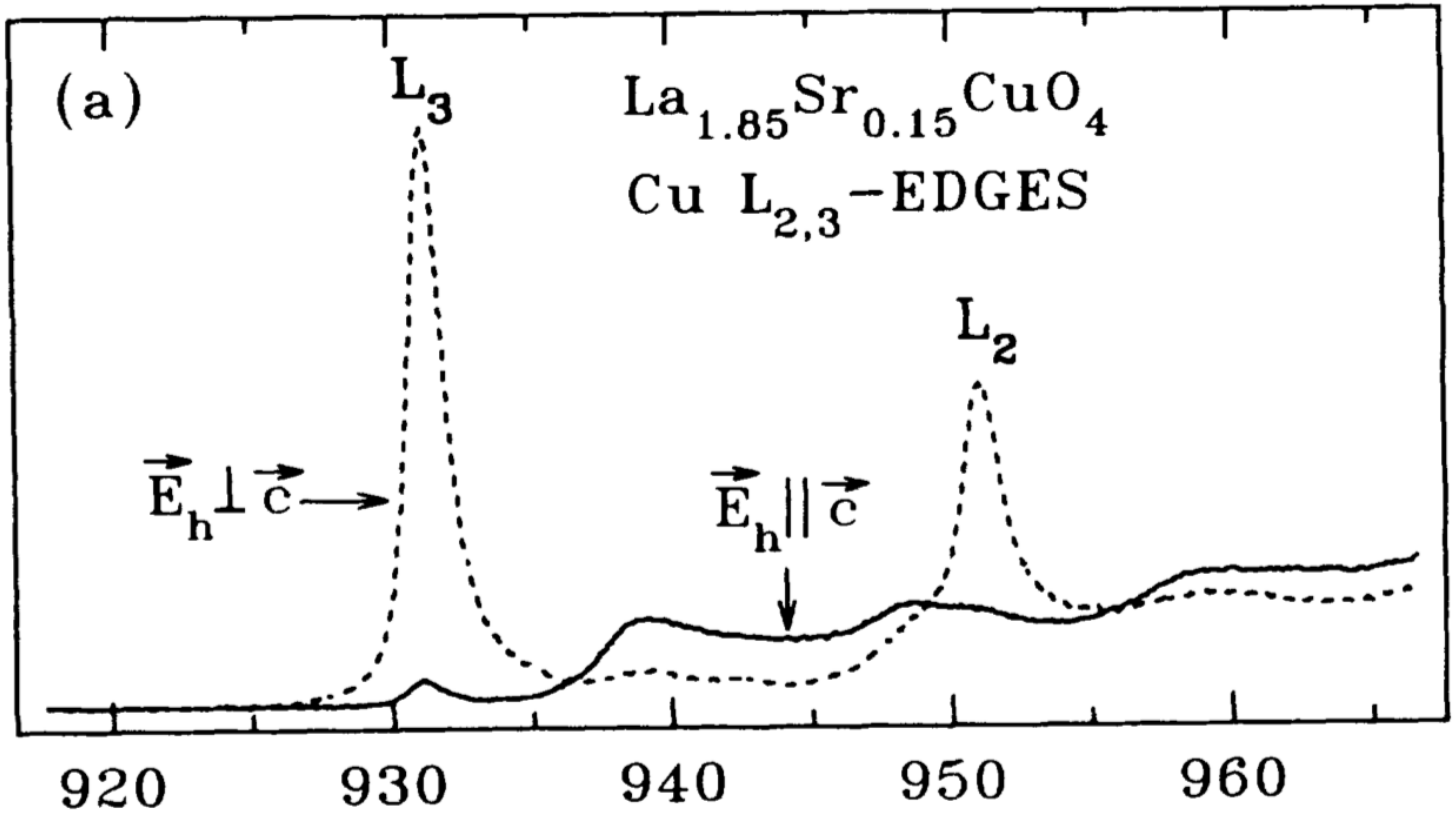
Character table for point group D_4

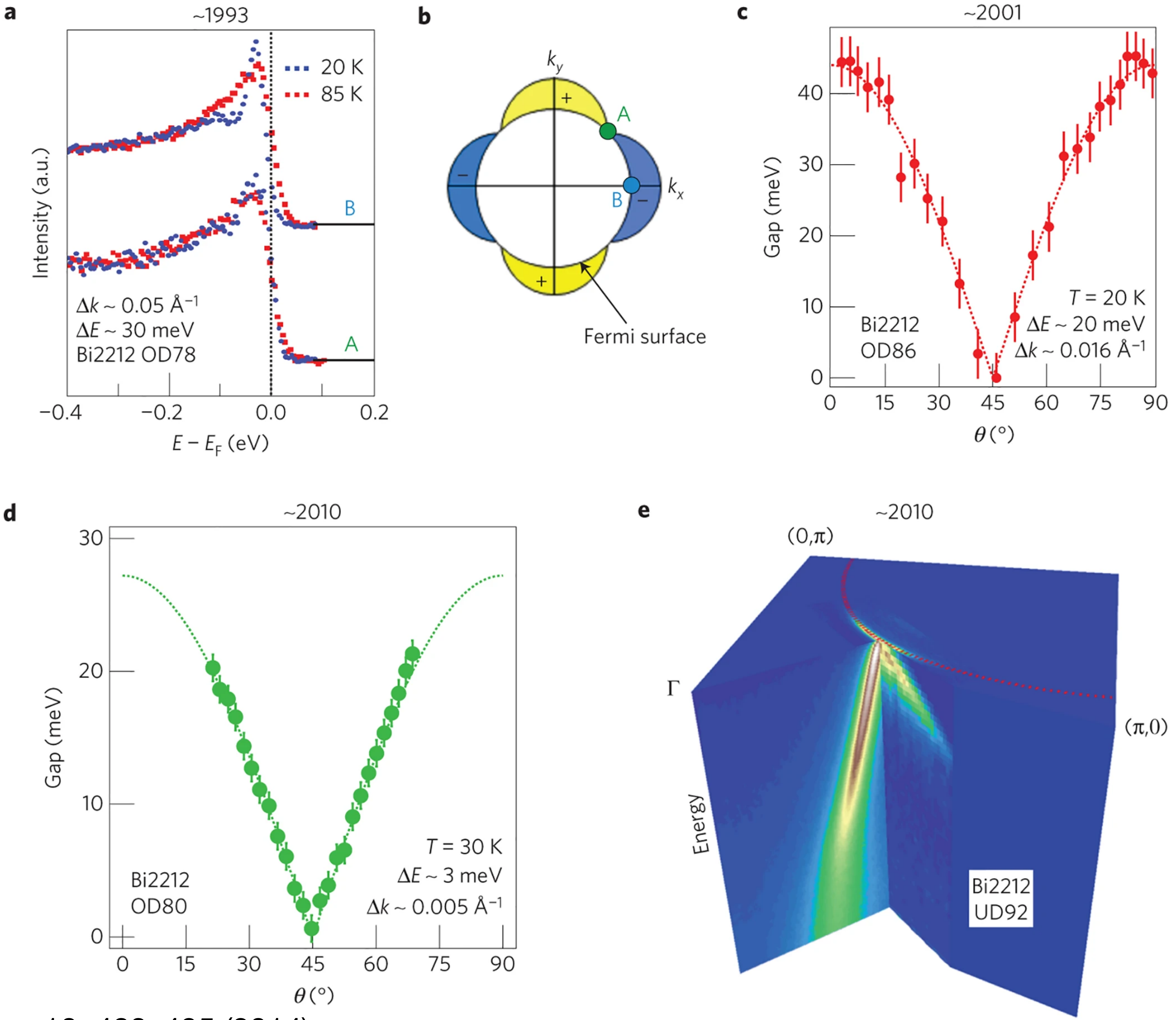
D_4	E	$2C_4$ (z)	C_2 (z)	$2C'_2$	$2C''_2$	linear functions, rotations	quadratic functions	cubic functions
A_1	+1	+1	+1	+1	+1	-	x^2+y^2, z^2	-
A_2	+1	+1	+1	-1	-1	z, R_z	-	$z^3, z(x^2+y^2)$
B_1	+1	-1	+1	+1	-1	-	x^2-y^2	xyz
B_2	+1	-1	+1	-1	+1	-	xy	$z(x^2-y^2)$
E	+2	0	-2	0	0	(x, y) (R_x, R_y)	(xz, yz)	(xz^2, yz^2) (xy^2, x^2y) (x^3, y^3)


ESRF

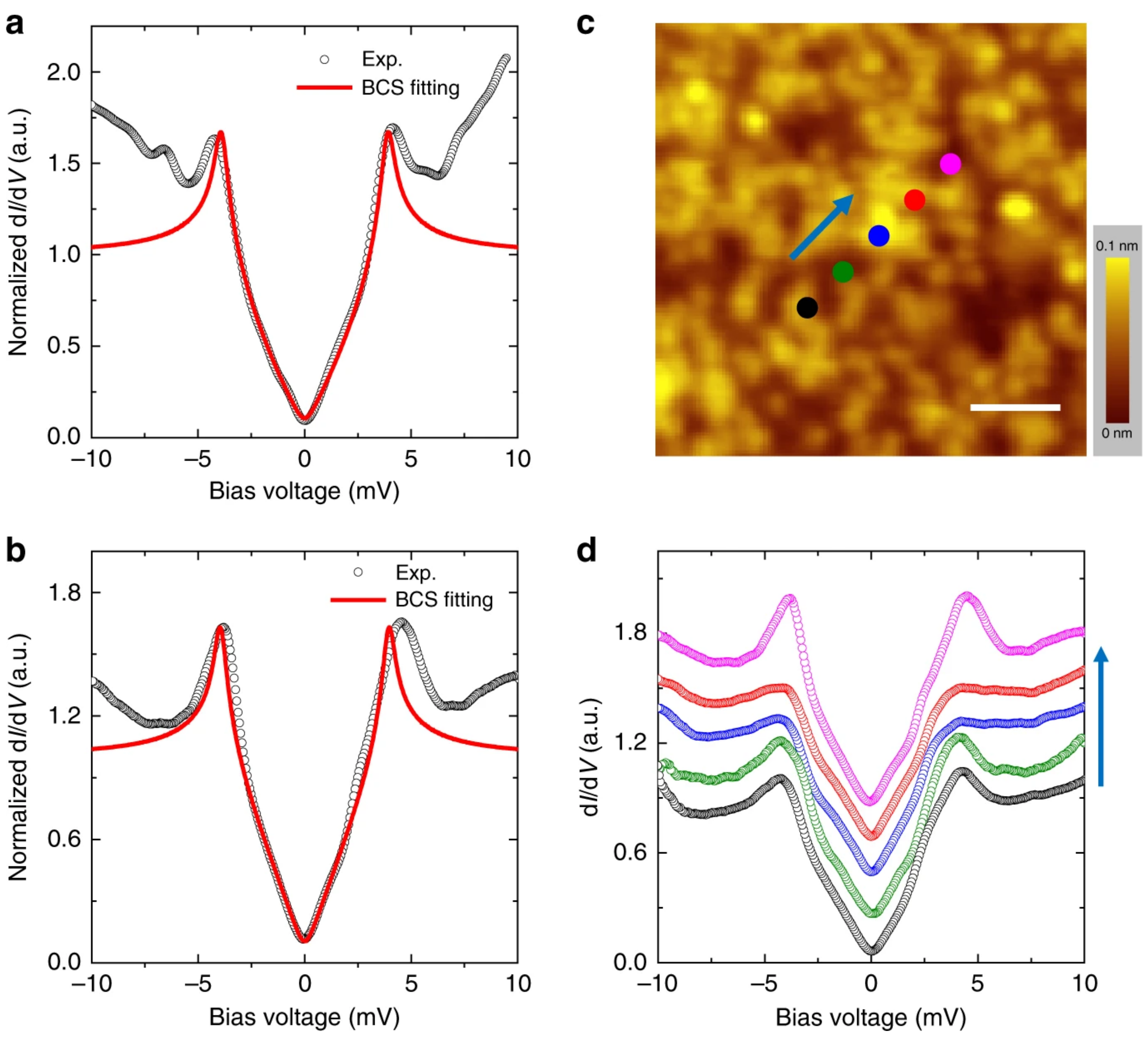

(a)
insertion device
beamline
optics
booster ring
bending magnet
linear accelerator
electron gun
e-
storage ring
(b)
N
S
e-
θ~1/γ
z
y
x
(c)
N
S
S
N
λID

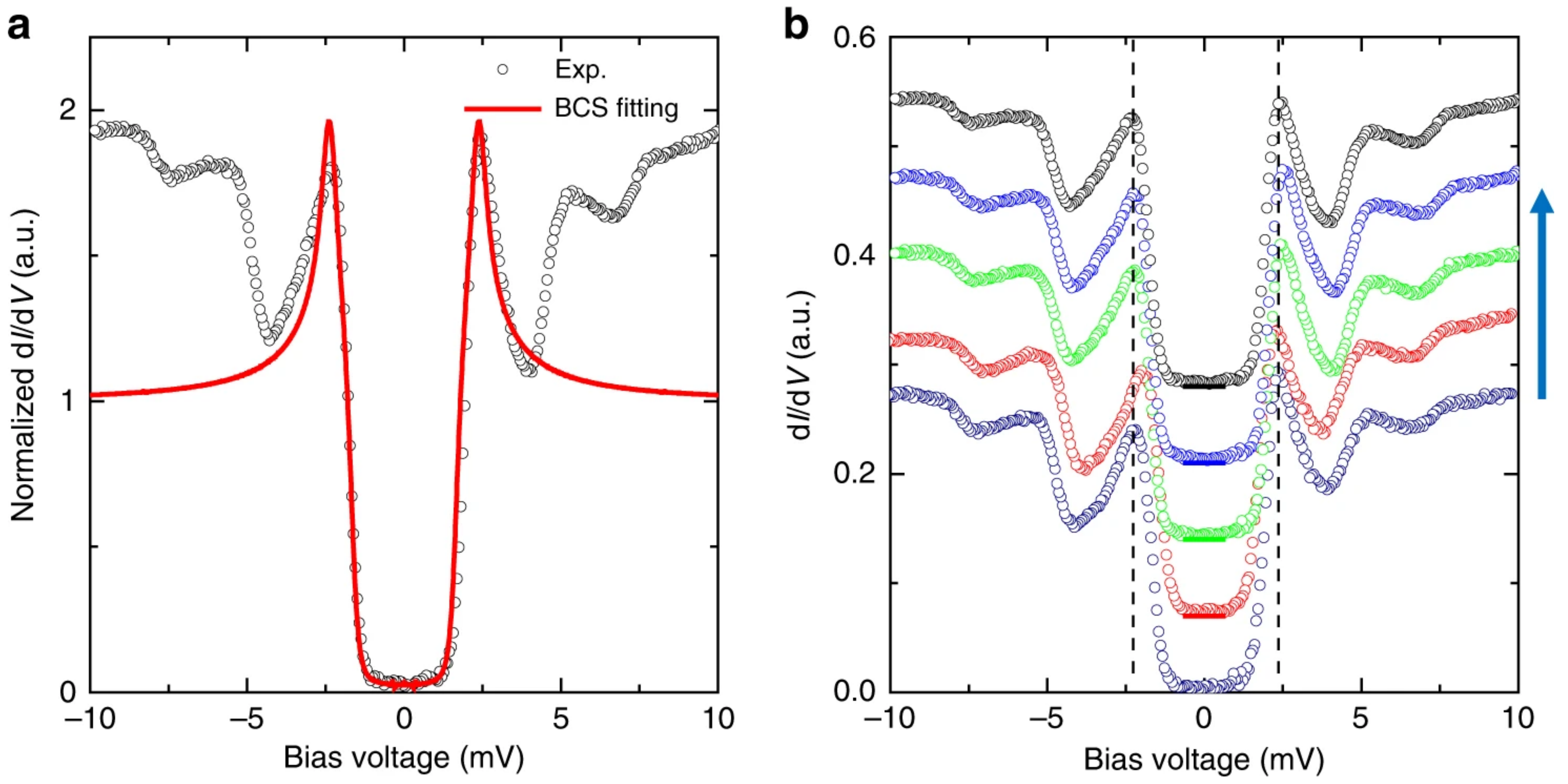

LaTiO3
VO
Cr2O3
MnO
FeO
CoO
NiO
CuO
Intensity (arb. units)
400
500
600
700
800
900
Photon energy (eV)


(a)
L3
La1.85Sr0.15CuO4
Cu L2,3-EDGES
L2
Eh ⊥ c
Eh || c
920
930
940
950
960



Hashimoto, Nature Physics 10, 483–495 (2014)





Gu, Nature Communications 11, 6027 (2020)