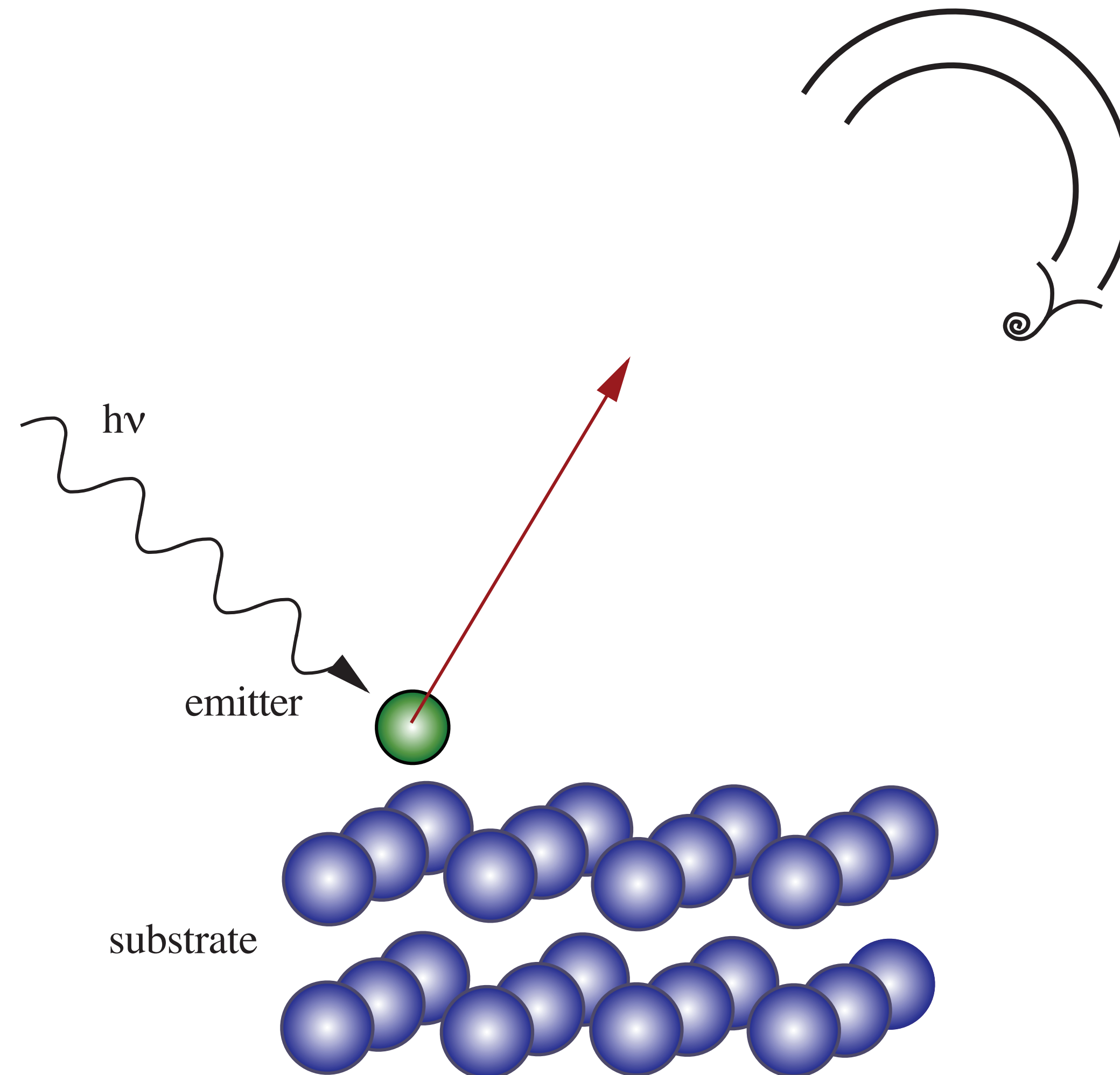


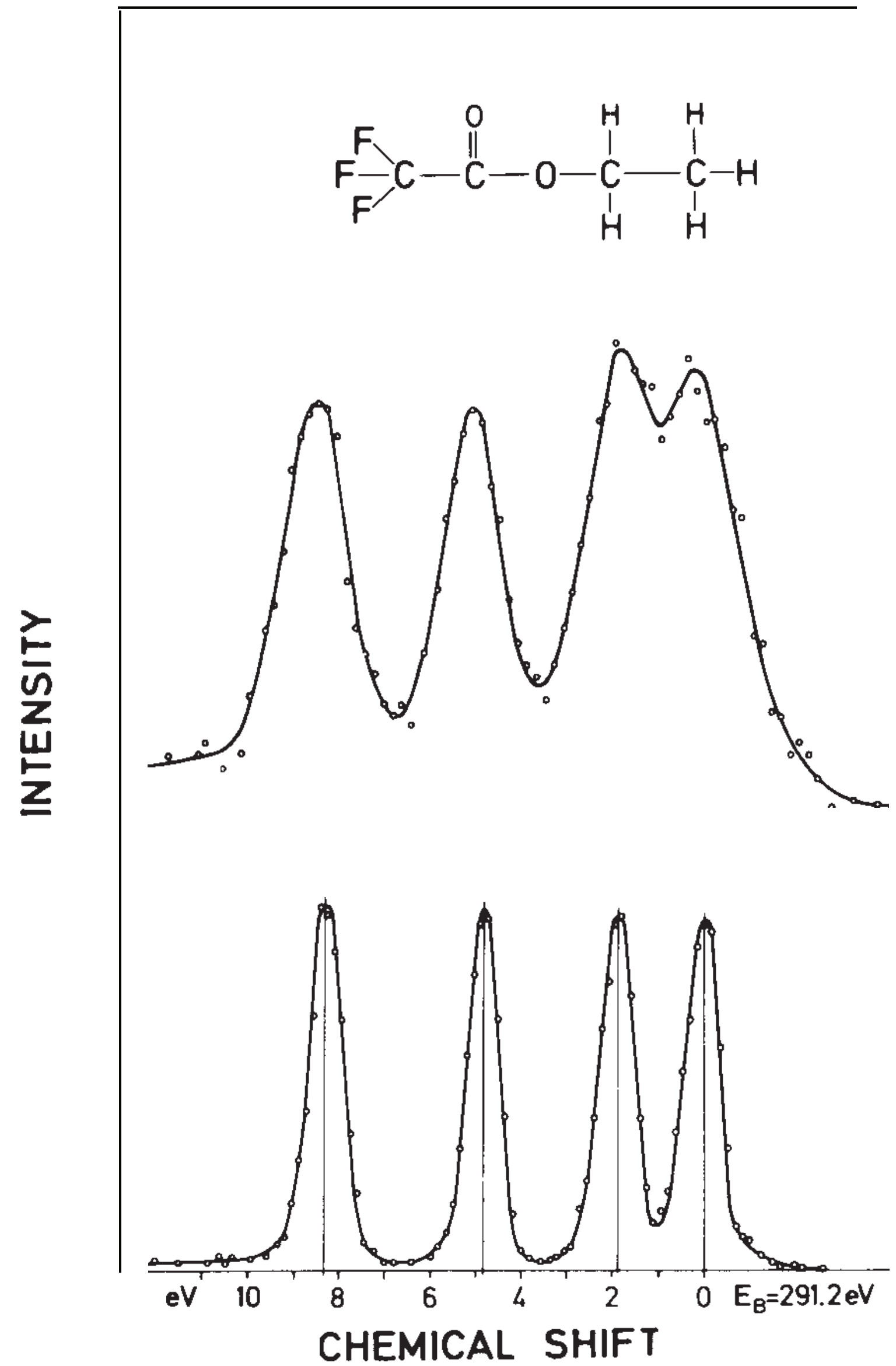


Ultrafast core level spectroscopy on FELs: XPS and XPD



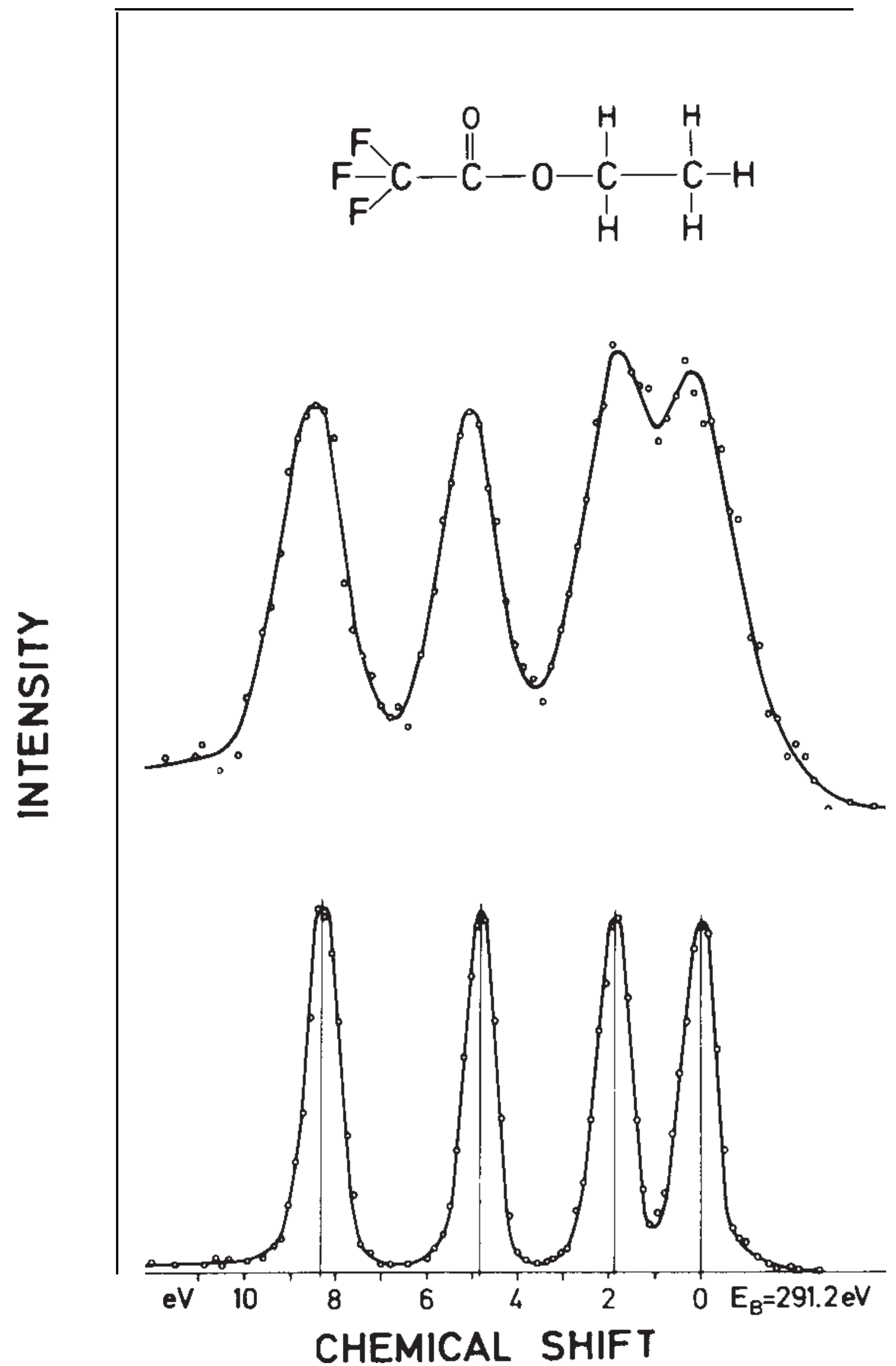


XPS: chemical sensitivity and many-body effects

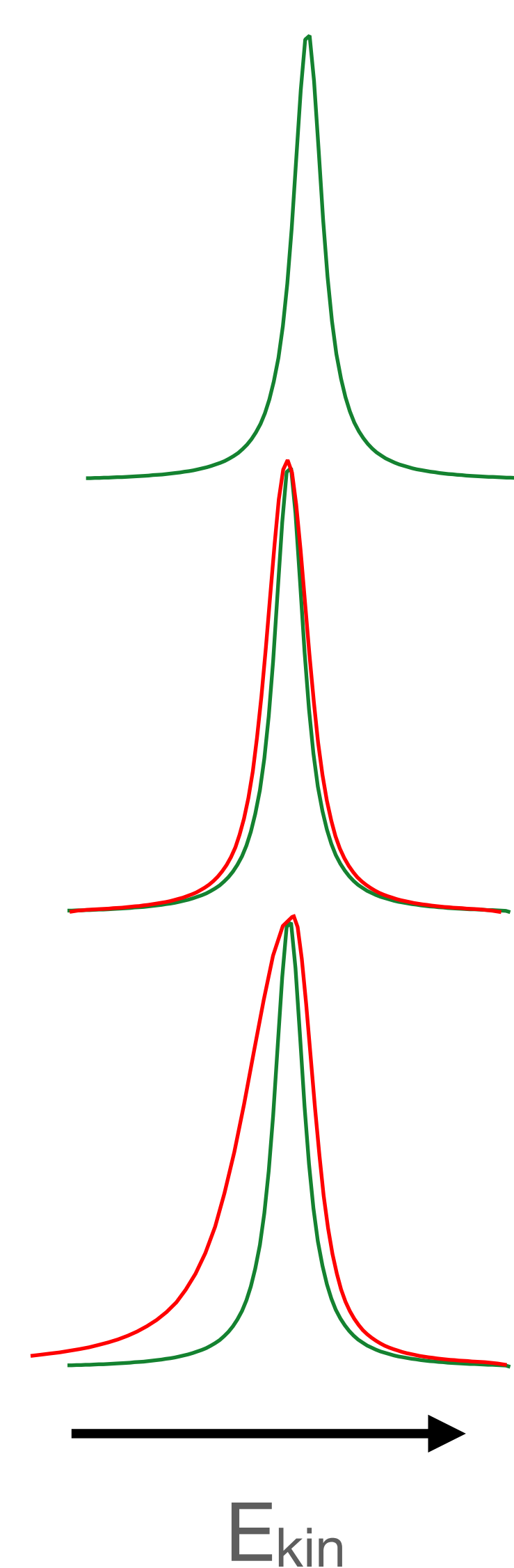




XPS: chemical sensitivity and many-body effects



U. Gelius, *et al.* J. Electron Spectrosc. Relat. Phenom. **2**, 405 (1973)



Lorentzian line shape (lifetime)

$$I = \frac{A}{(\omega - \omega_0)^2 + C}$$

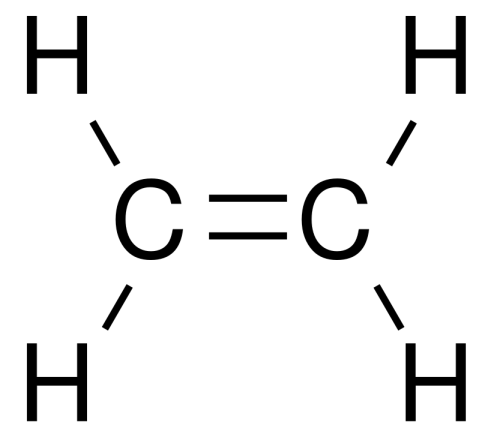
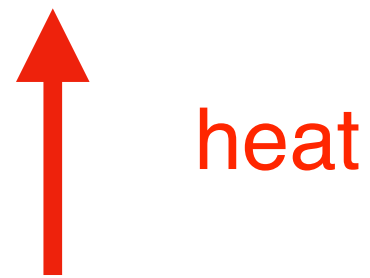
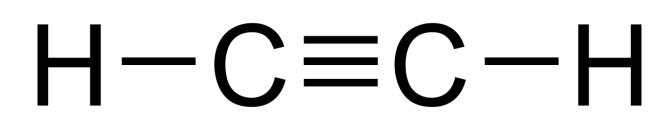
broadening by phonons
in the excitation process
(Lorentzian convoluted with Gaussian)

for metals: asymmetric because
of electron-hole pair excitations
(Doniach-Sunjic)

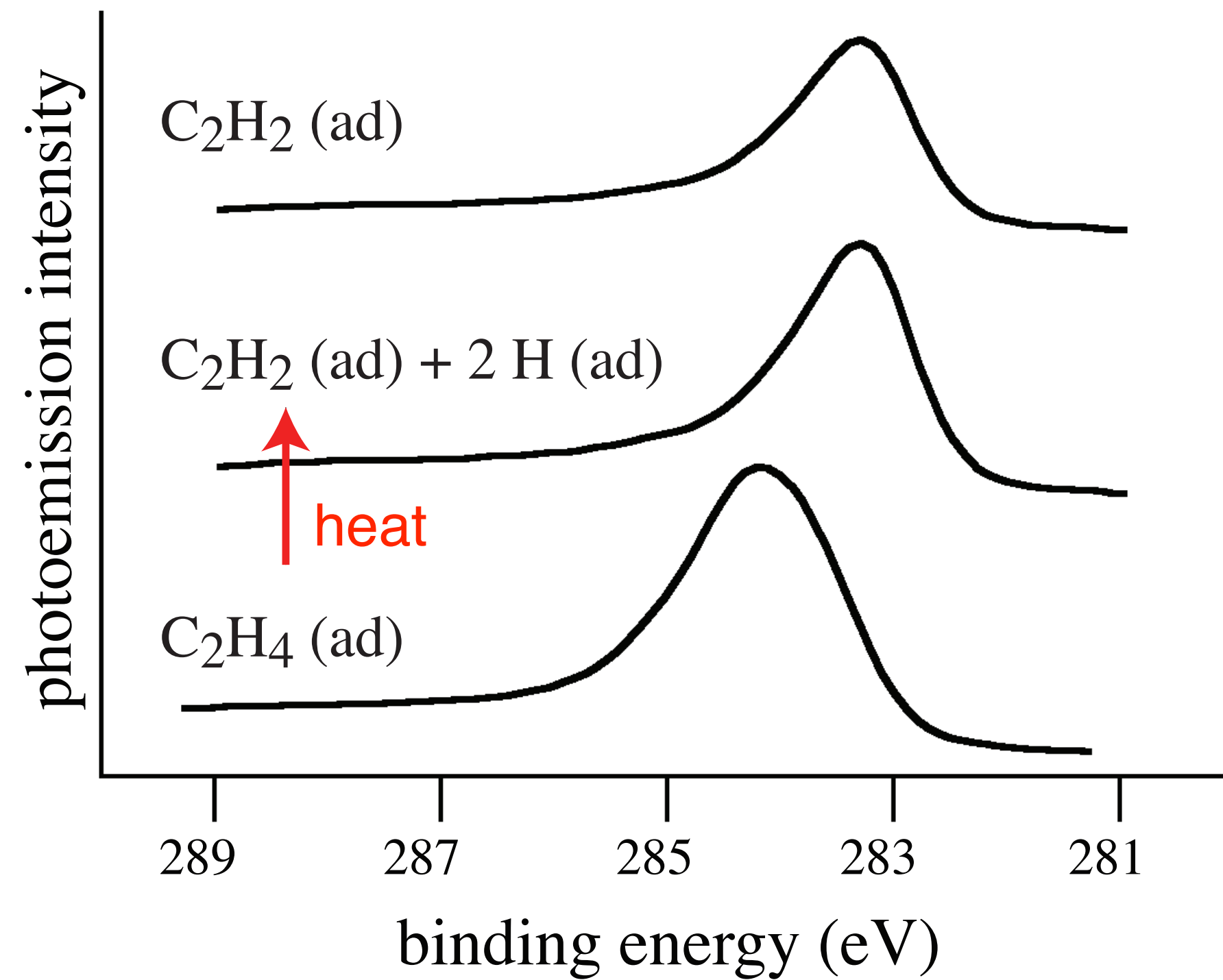
P. H. Citrin *et al.*, Phys. Rev. B **16**, 4256 (1977)



Following the geometrical changes in a surface reaction: Dehydration of Ethylene on Ni(111)



C 1s XPS

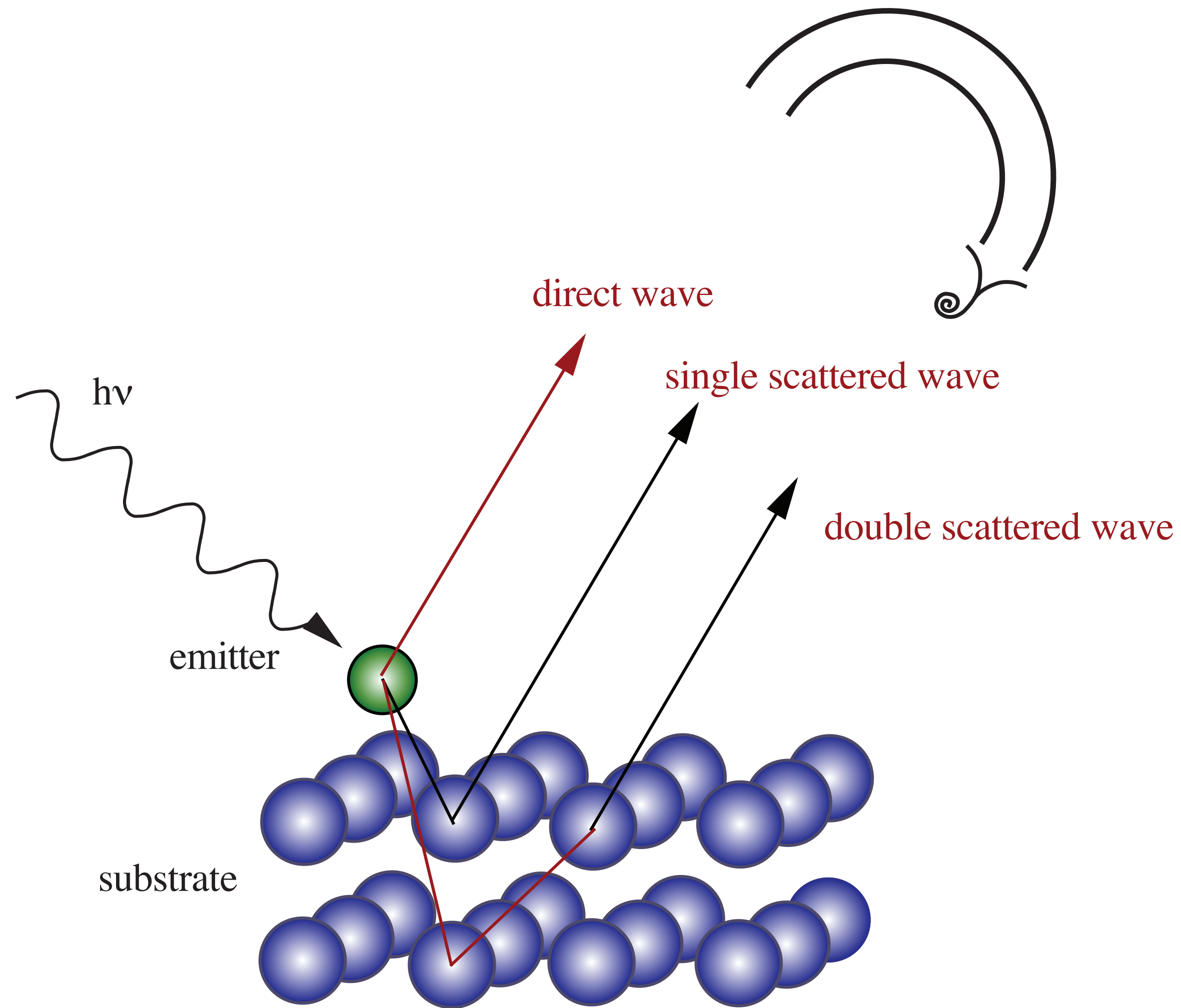


J. E. Demuth and D. A. Eastman, Phys. Rev. Lett. **32**, 1123 (1974)

S. Bao, Ph. Hofmann, K.-M. Schindler, V. Fritzsche, A. M. Bradshaw, D. P. Woodruff, C. Casado and M. C. Asensio, J. Phys.: Condens. Matter **6** L93, (1994).

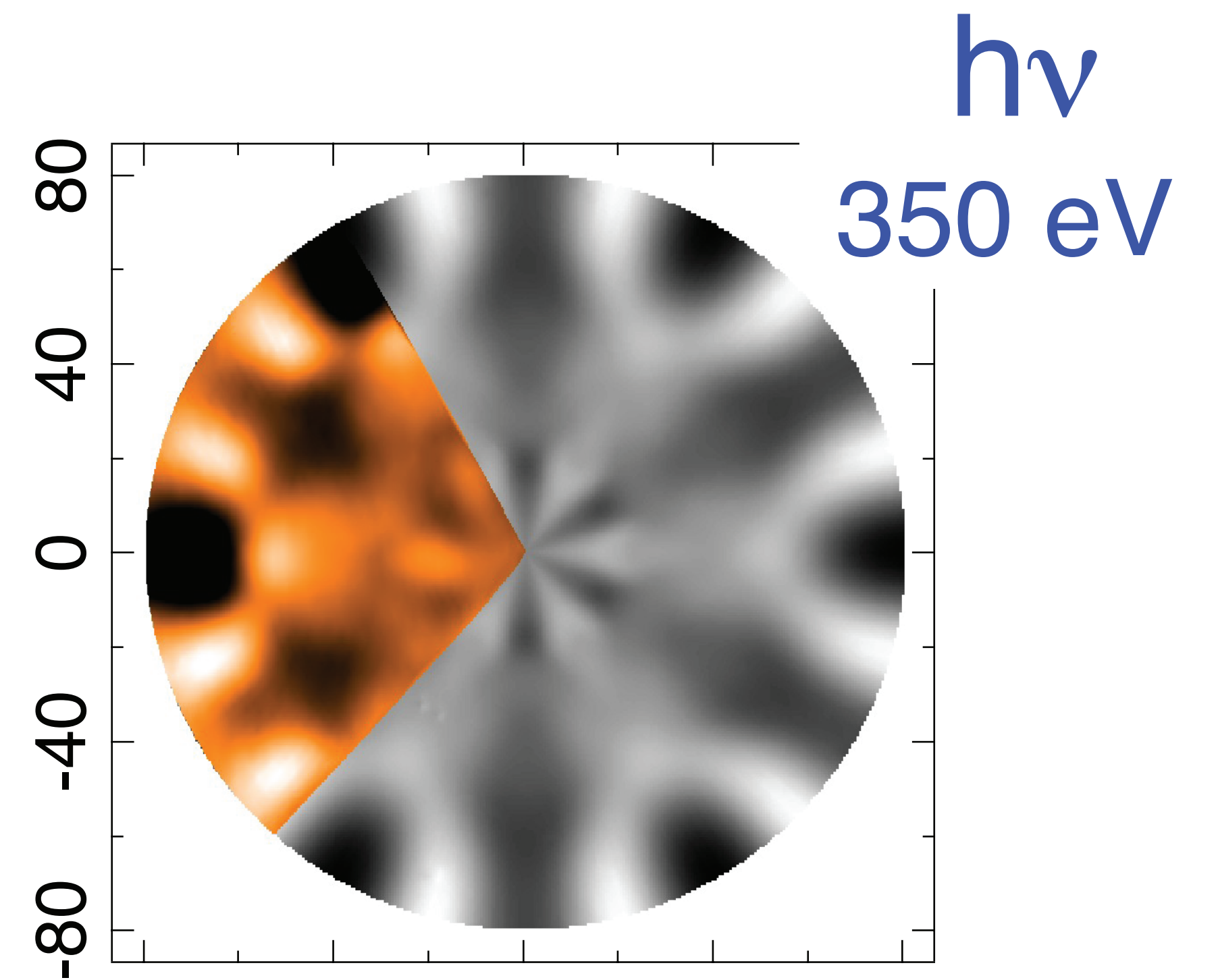
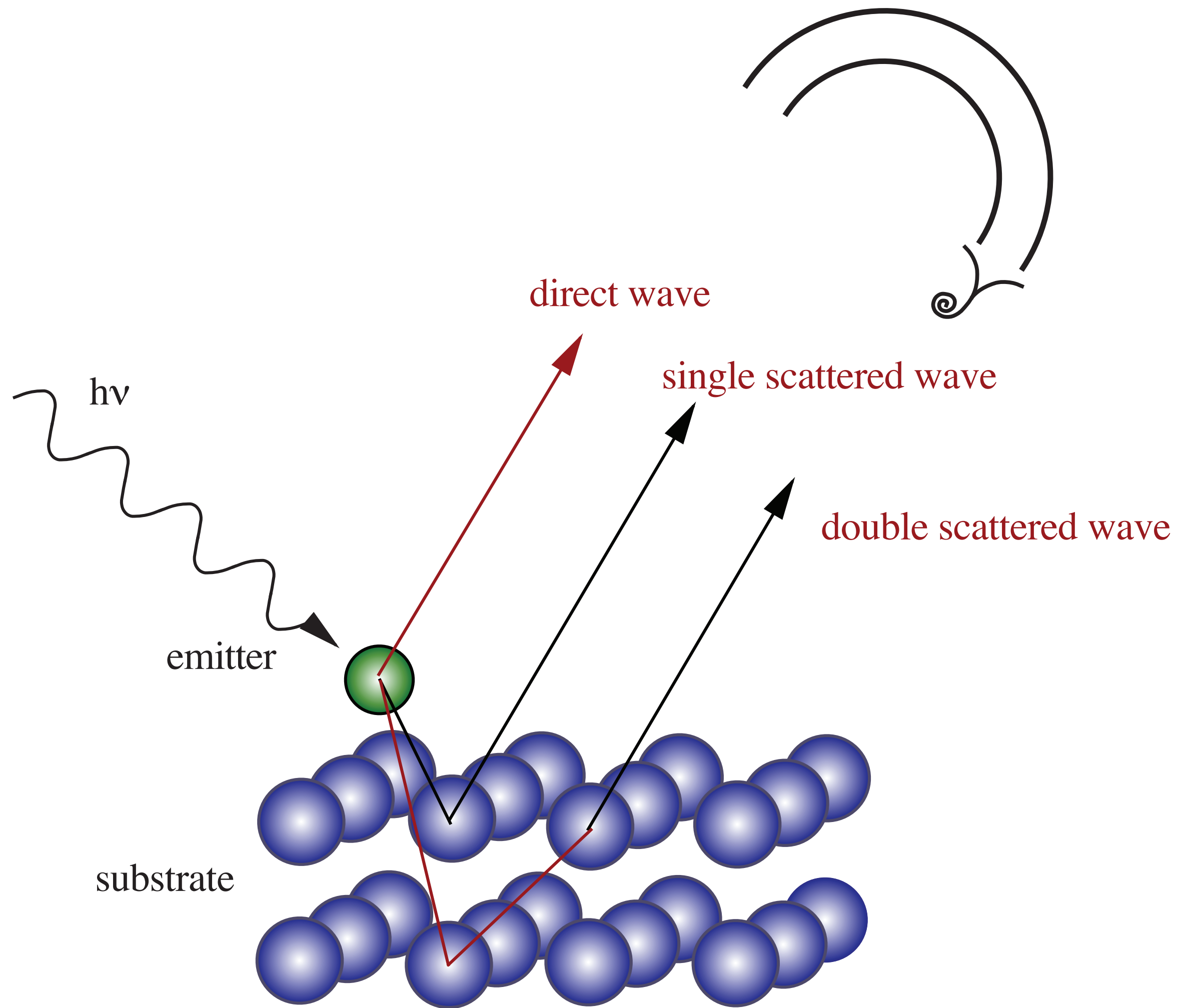


X-ray Photoelectron Diffraction (XPD, PhD)



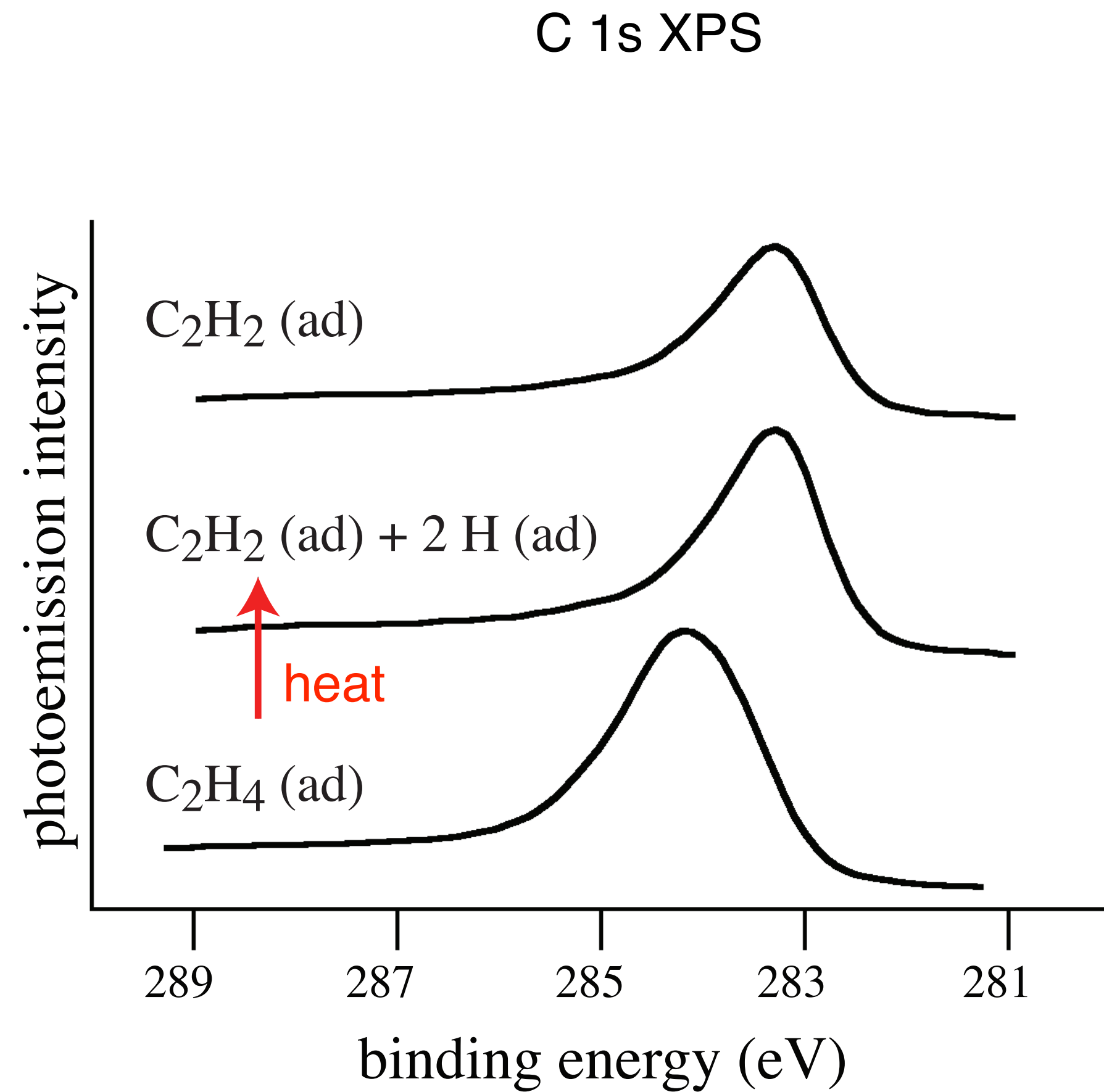


X-ray Photoelectron Diffraction (XPD, PhD)





Following the geometrical changes in a surface reaction: Dehydration of Ethylene on Ni(111)

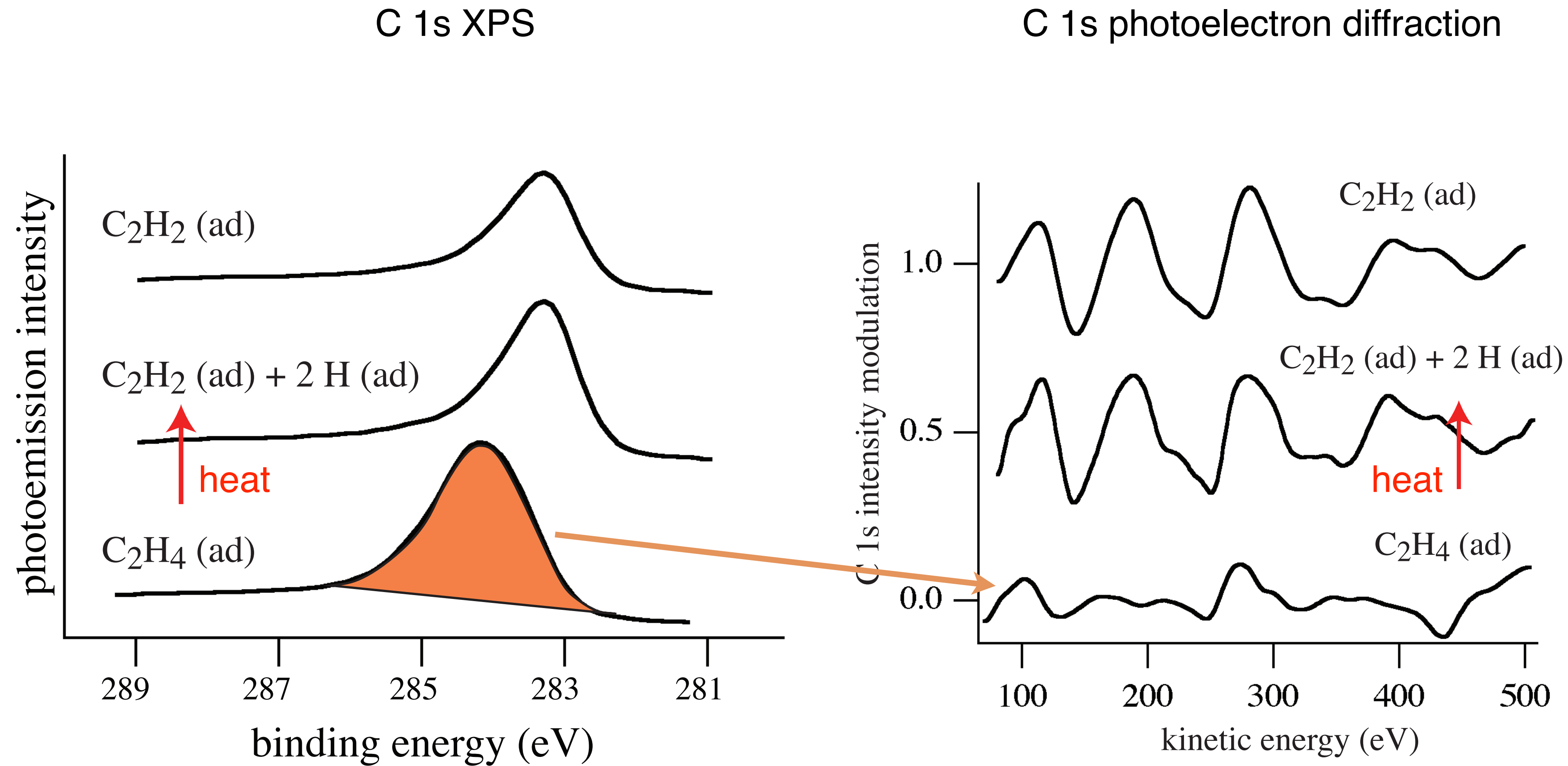


S. Bao, Ph. Hofmann, K.-M. Schindler, V. Fritzsche, A. M. Bradshaw, D. P. Woodruff, C. Casado and M. C. Asensio,
J. Phys.: Condens. Matter **6** L93, (1994).

see also J. E. Demuth and D. A. Eastman, Phys. Rev. Lett. **32**, 1123 (1974)



Following the geometrical changes in a surface reaction: Dehydration of Ethylene on Ni(111)

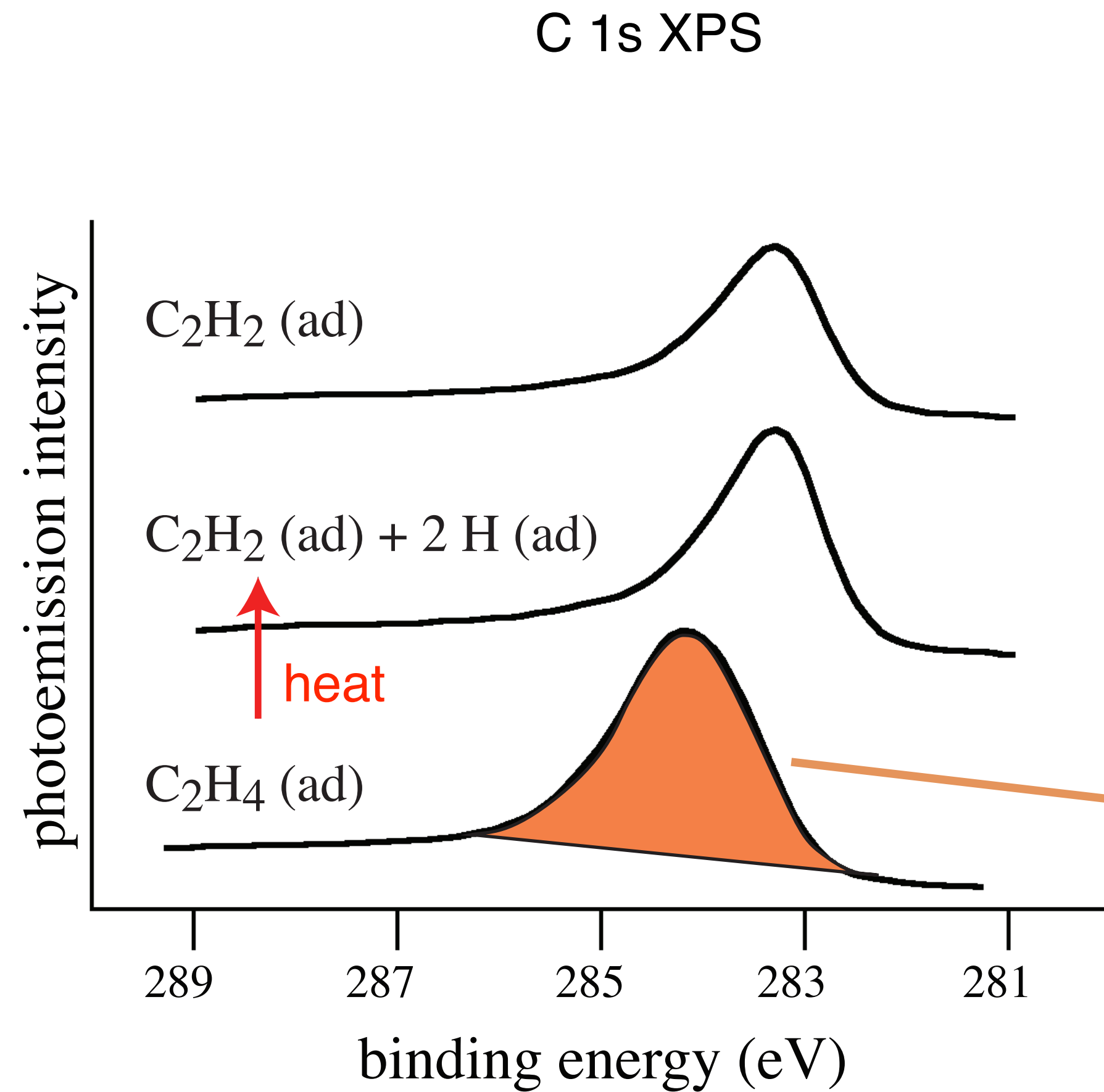


S. Bao, Ph. Hofmann, K.-M. Schindler, V. Fritzsche, A. M. Bradshaw, D. P. Woodruff, C. Casado and M. C. Asensio,
J. Phys.: Condens. Matter **6** L93, (1994).

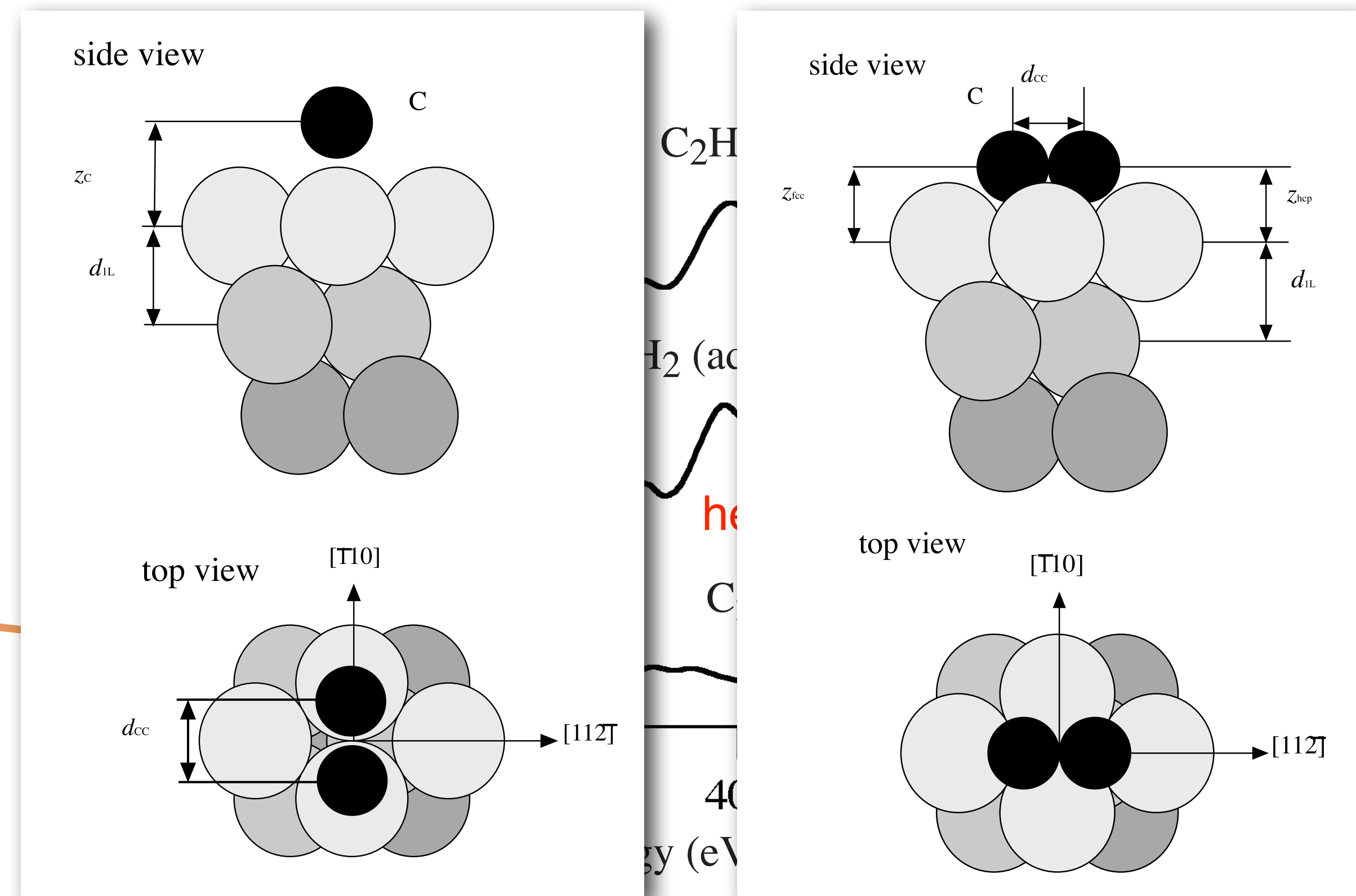
see also J. E. Demuth and D. A. Eastman, Phys. Rev. Lett. **32**, 1123 (1974)



Following the geometrical changes in a surface reaction: Dehydration of Ethylene on Ni(111)



C 1s photoelectron diffraction

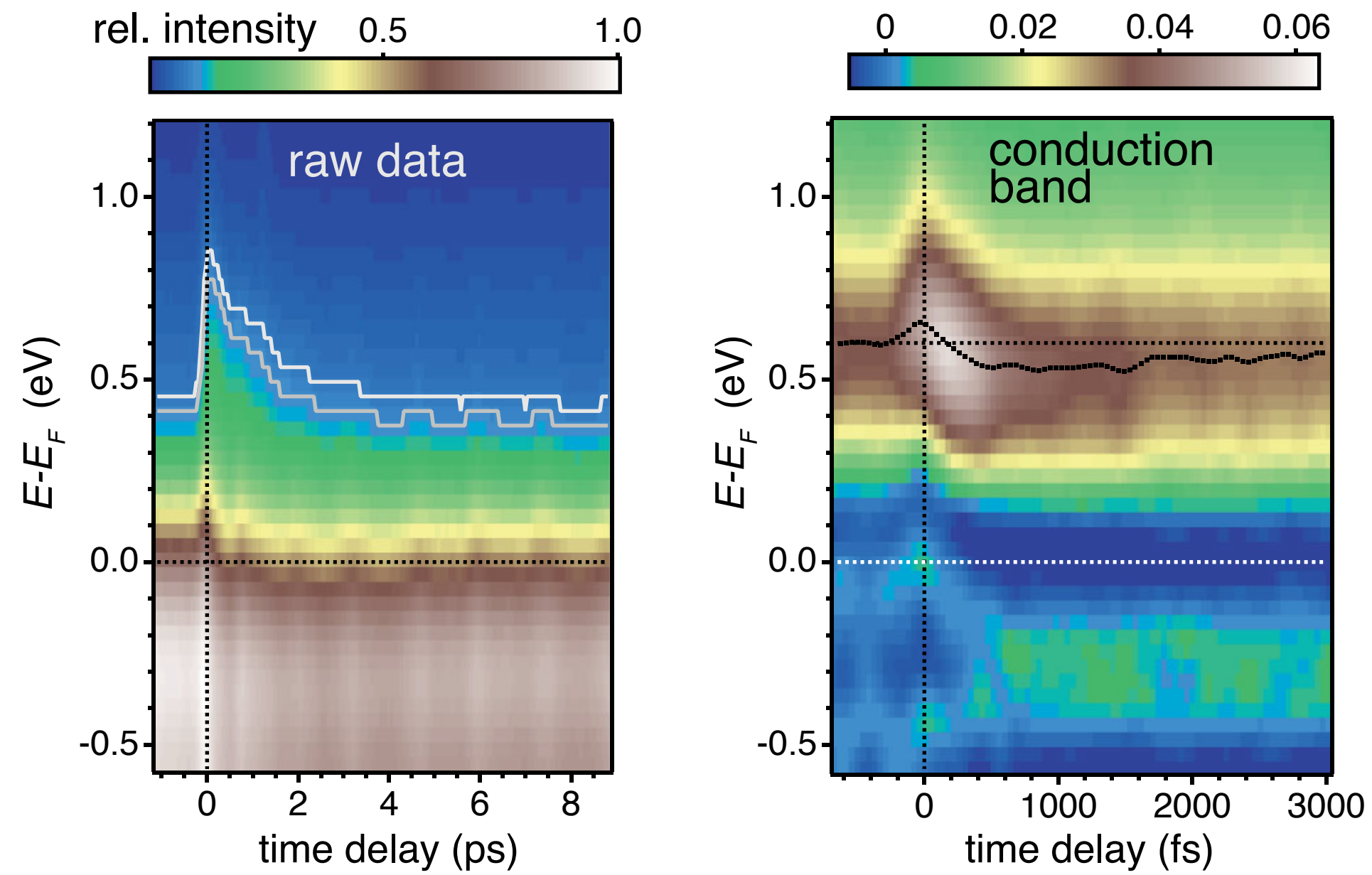


S. Bao, Ph. Hofmann, K.-M. Schindler, V. Fritzsche, A. M. Bradshaw, D. P. Woodruff, C. Casado and M. C. Asensio, J. Phys.: Condens. Matter **6** L93, (1994).

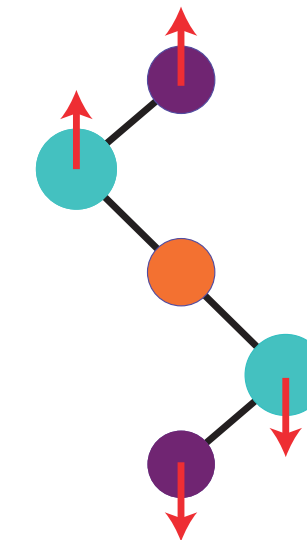
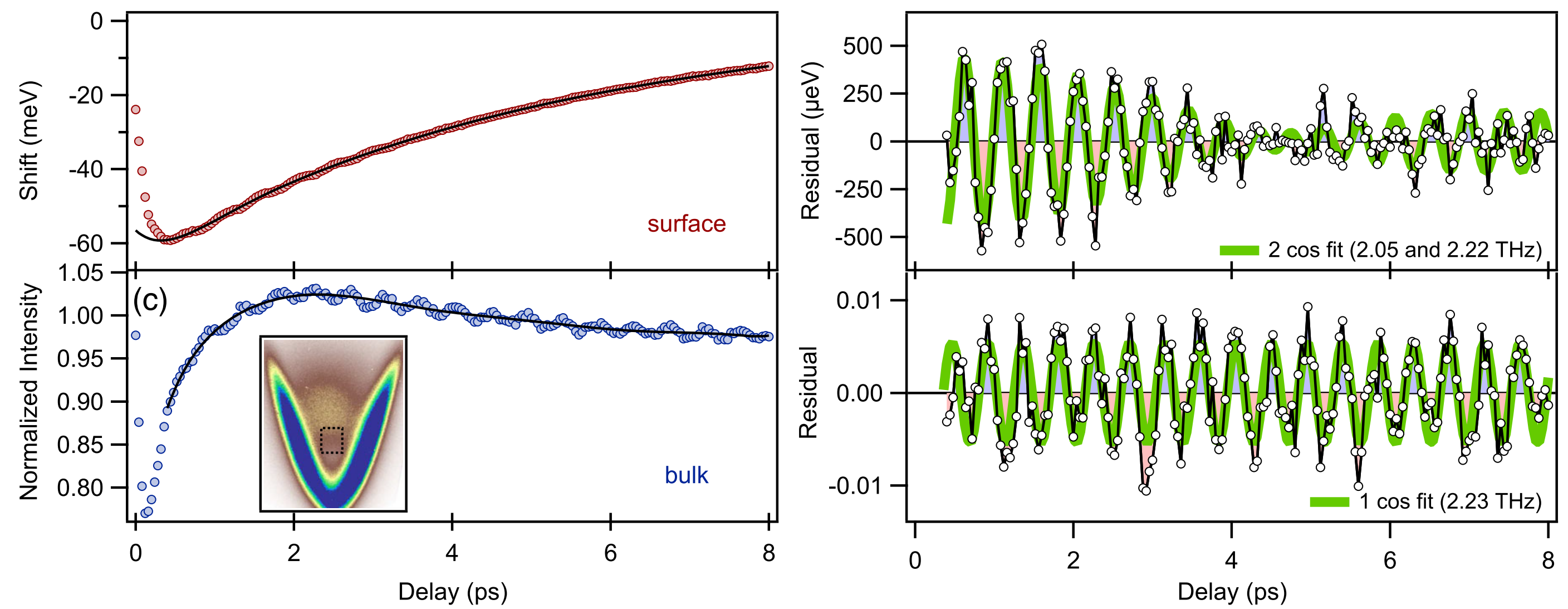
see also J. E. Demuth and D. A. Eastman, Phys. Rev. Lett. **32**, 1123 (1974)

Coherent phonons

on Bi(114)



on Bi_2Se_3



Leuenberger *et al.*, Phys. Rev. Lett. **110**, 136806 (2013)

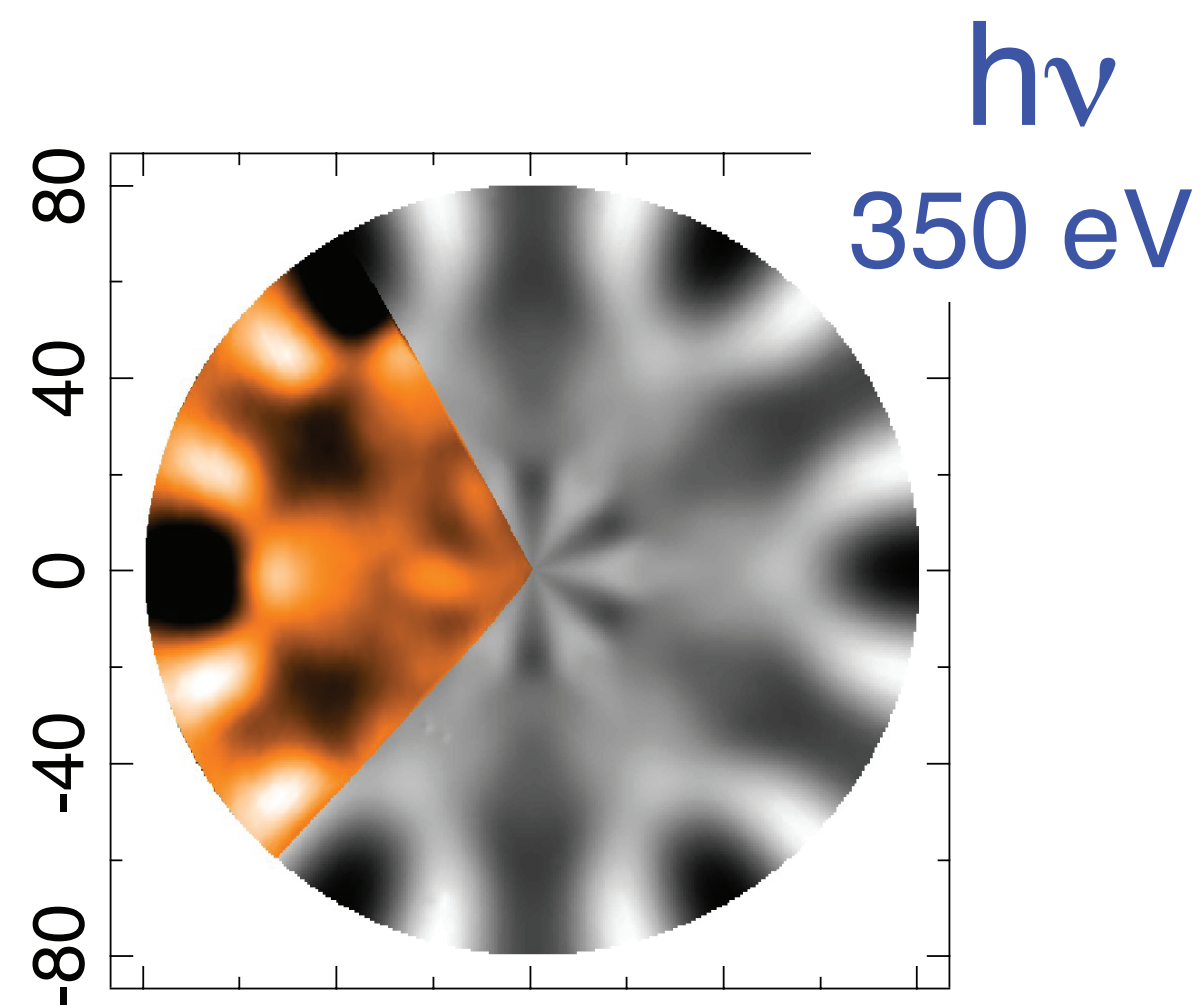
J. A. Sobota *et al.*, Phys. Rev. Lett. **113**, 157401 (2014)



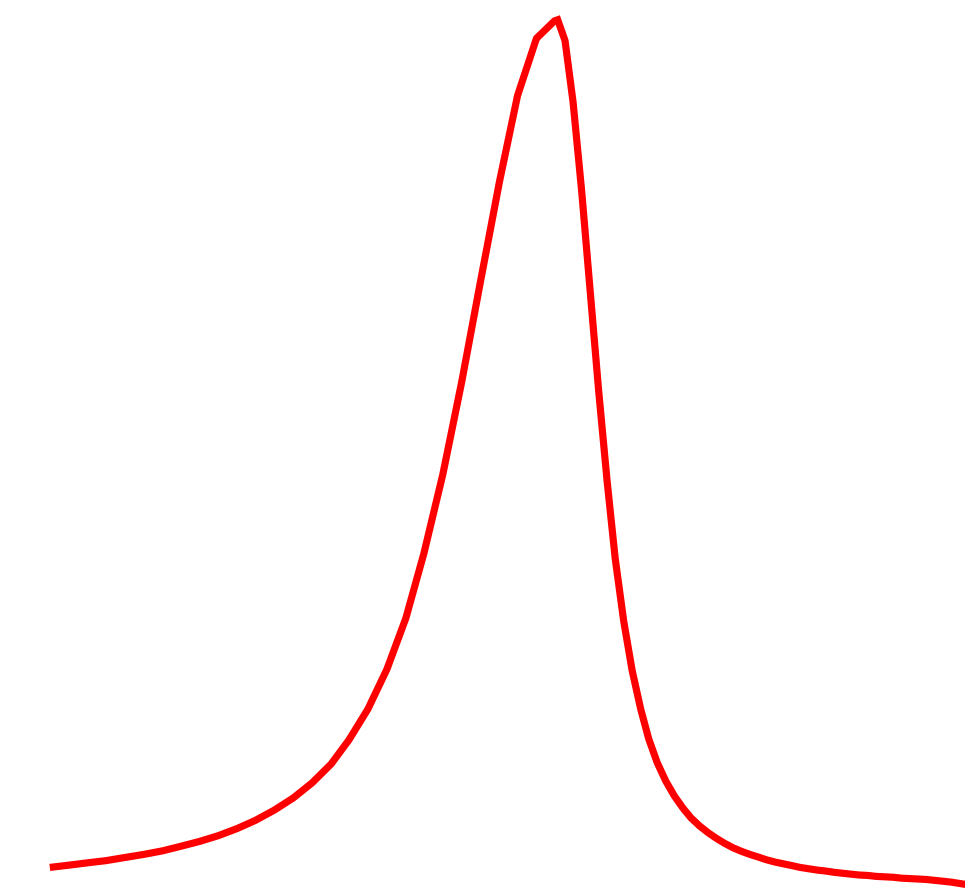
Ultrafast core level spectroscopy on FELs: XPS and XPD

- Track binding energy, lineshape and intensity, resolved in time and angle.
- Or at least:

intensity: angle-resolved, time-resolved

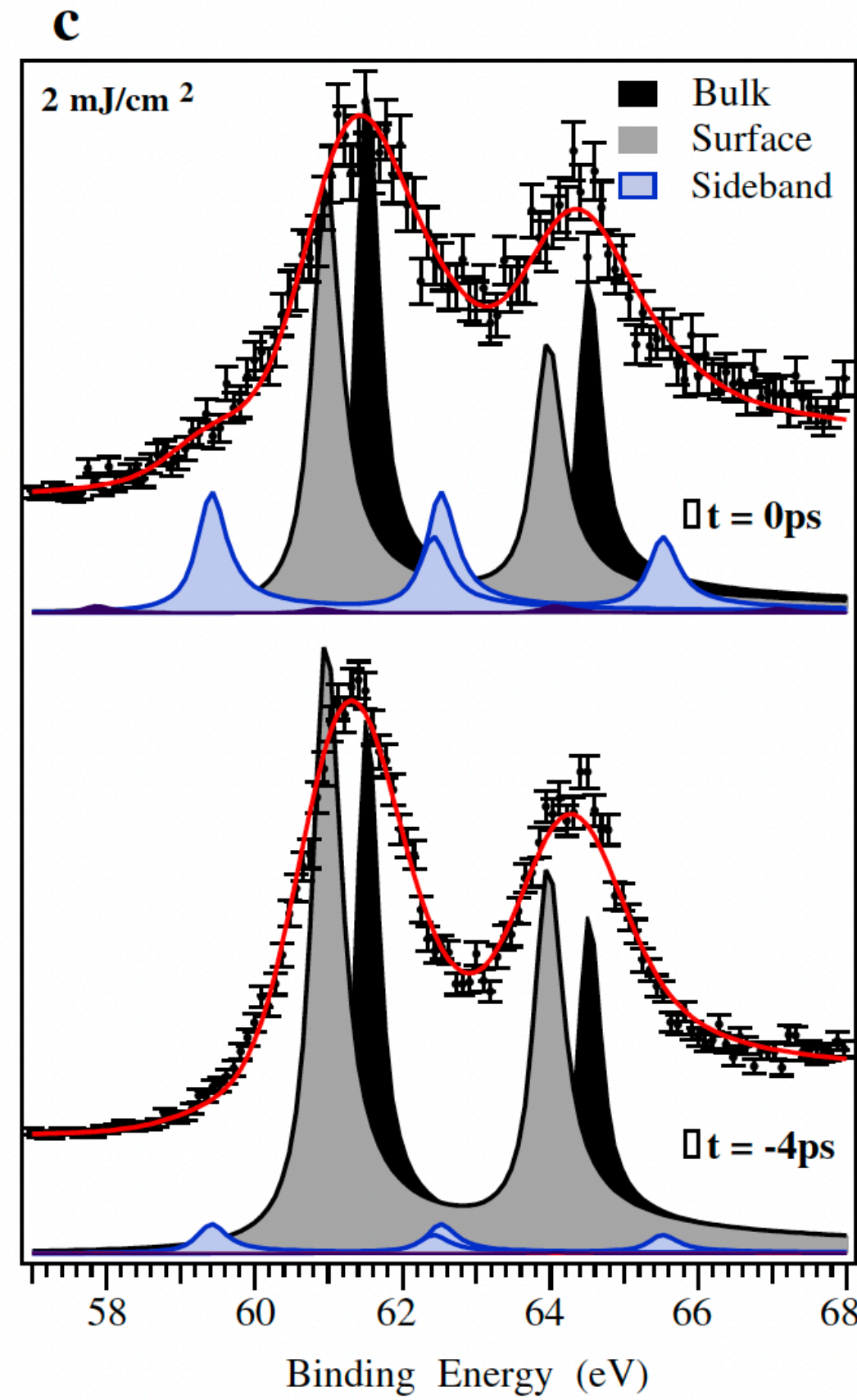
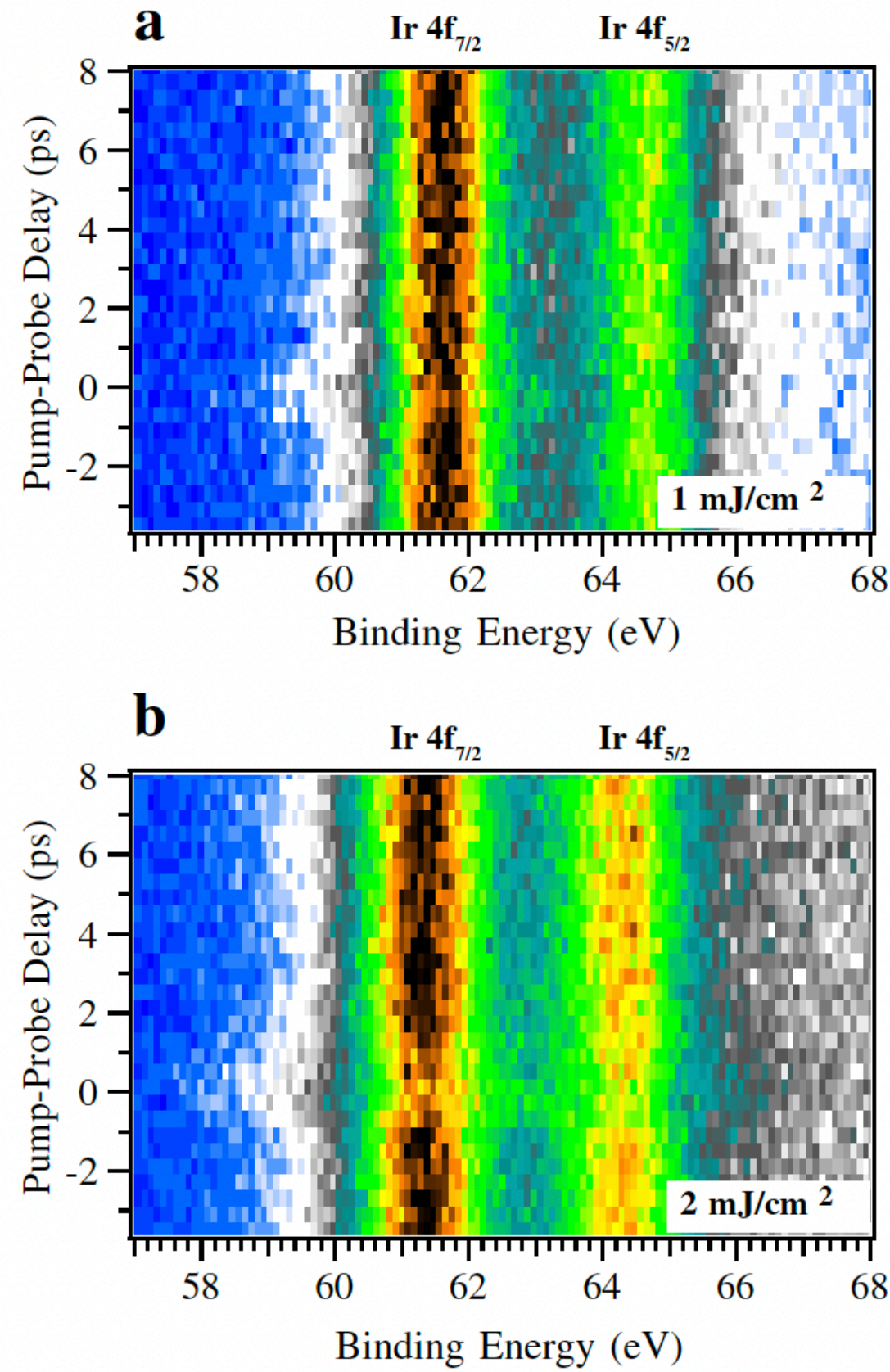


lineshape: time-resolved but angle-integrated



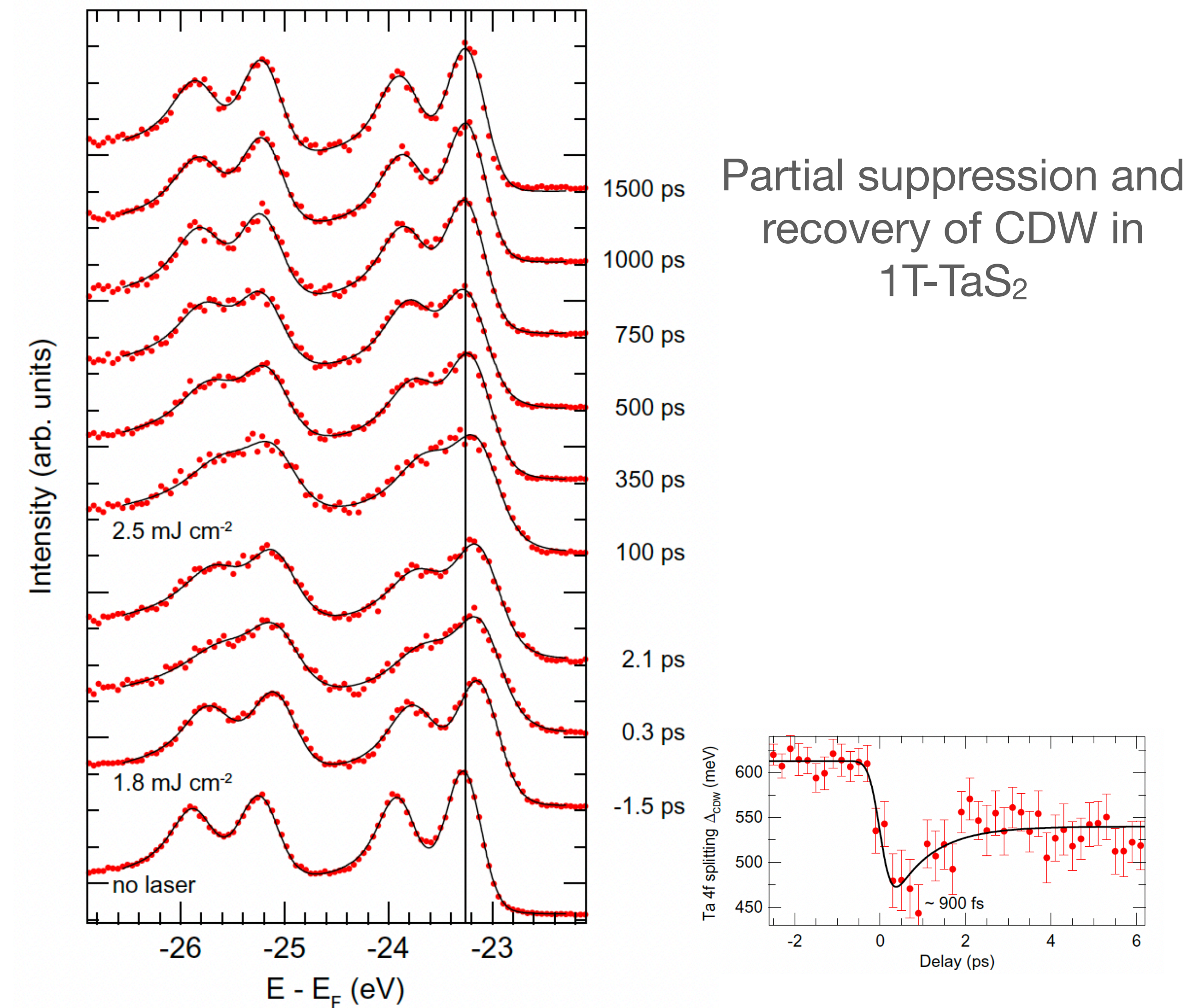


ultrafast XPS @ FLASH



- low repetition rate, inefficient electron detection, low count rate
- space charge

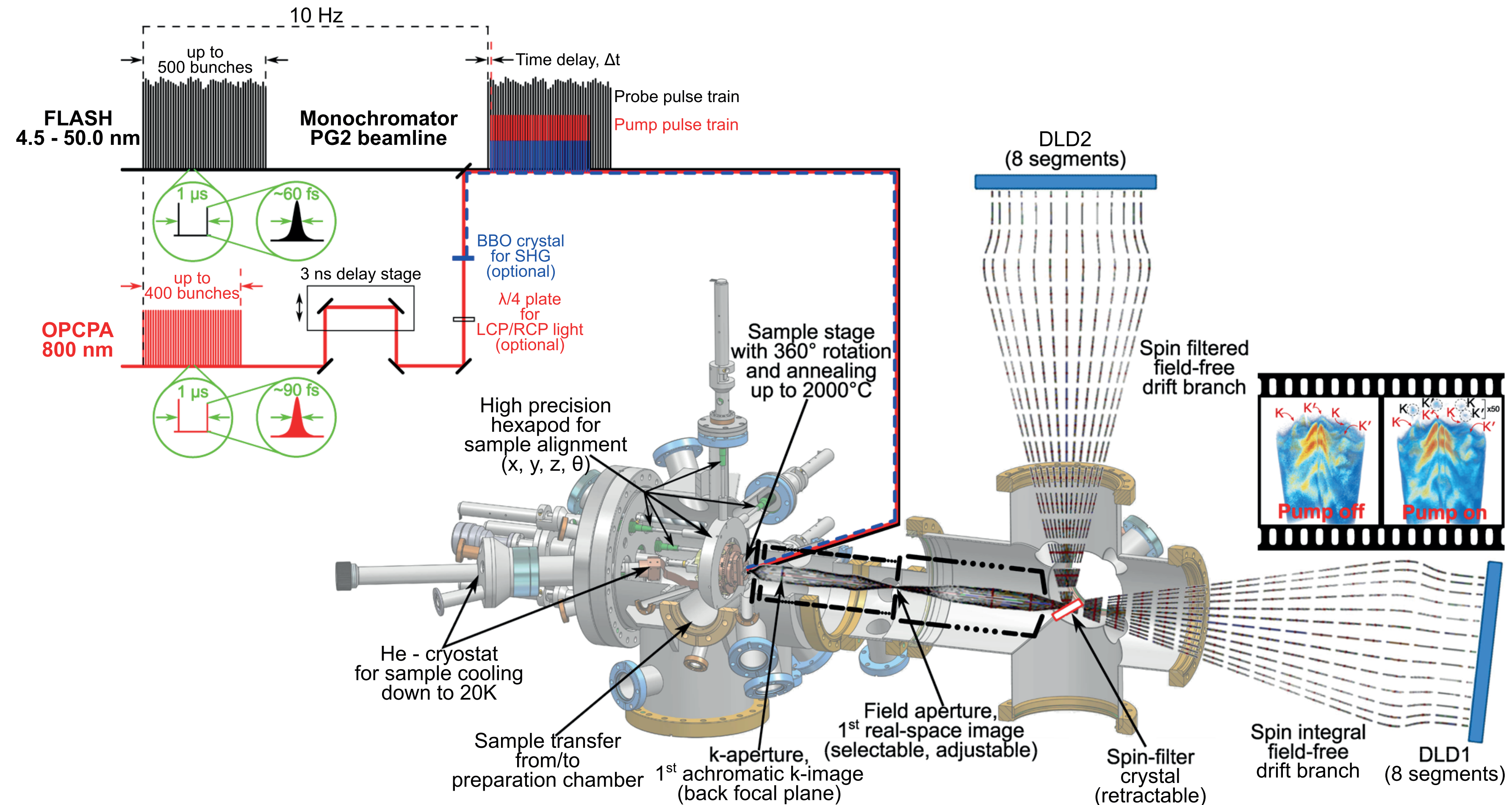
M. Dell'Angela *et al.*, Surf. Sci. **643**, 197 (2016)



S. Hellmann *et al.*, New Journal of Physics **14**, 013062 (2012)



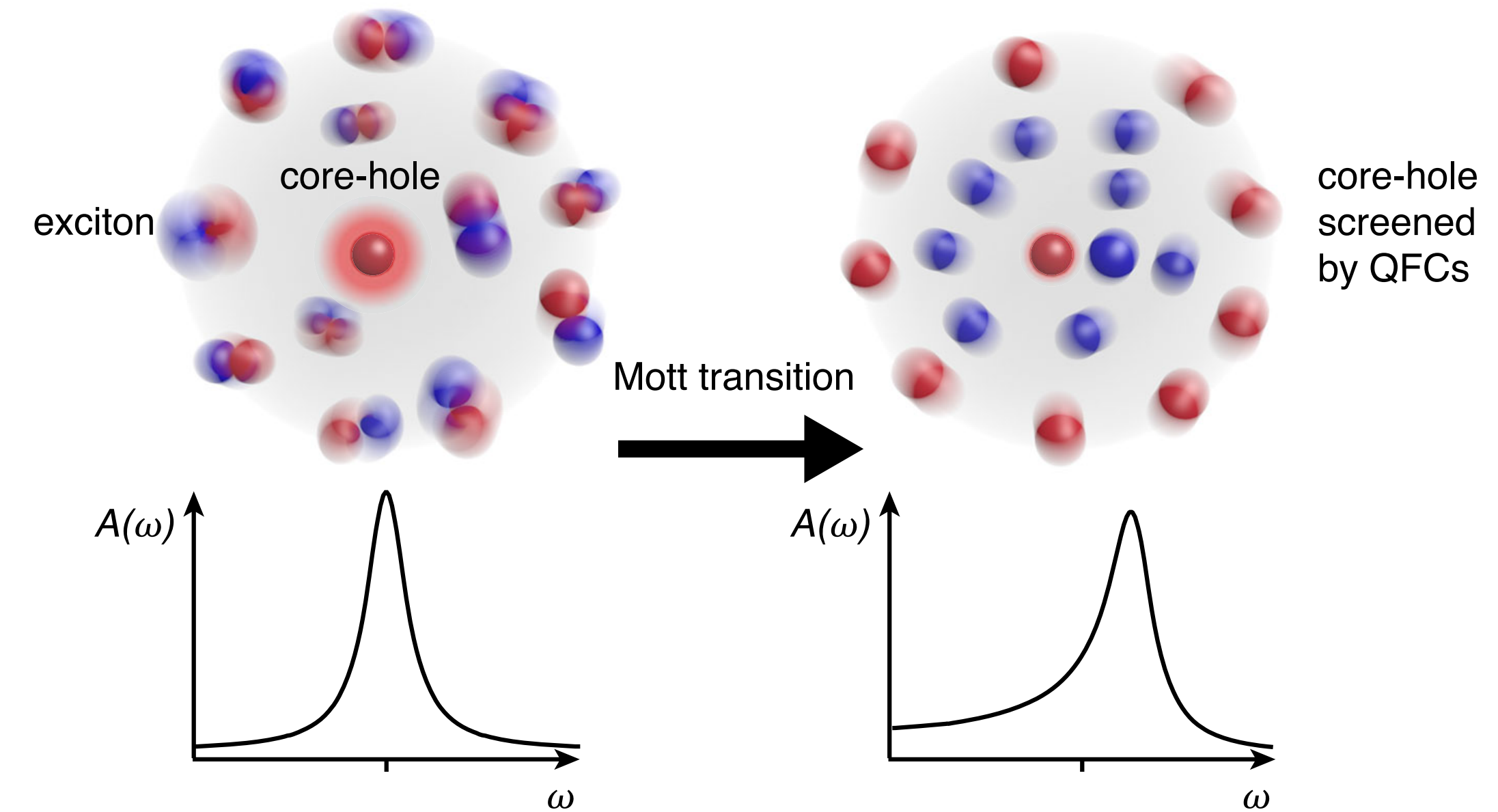
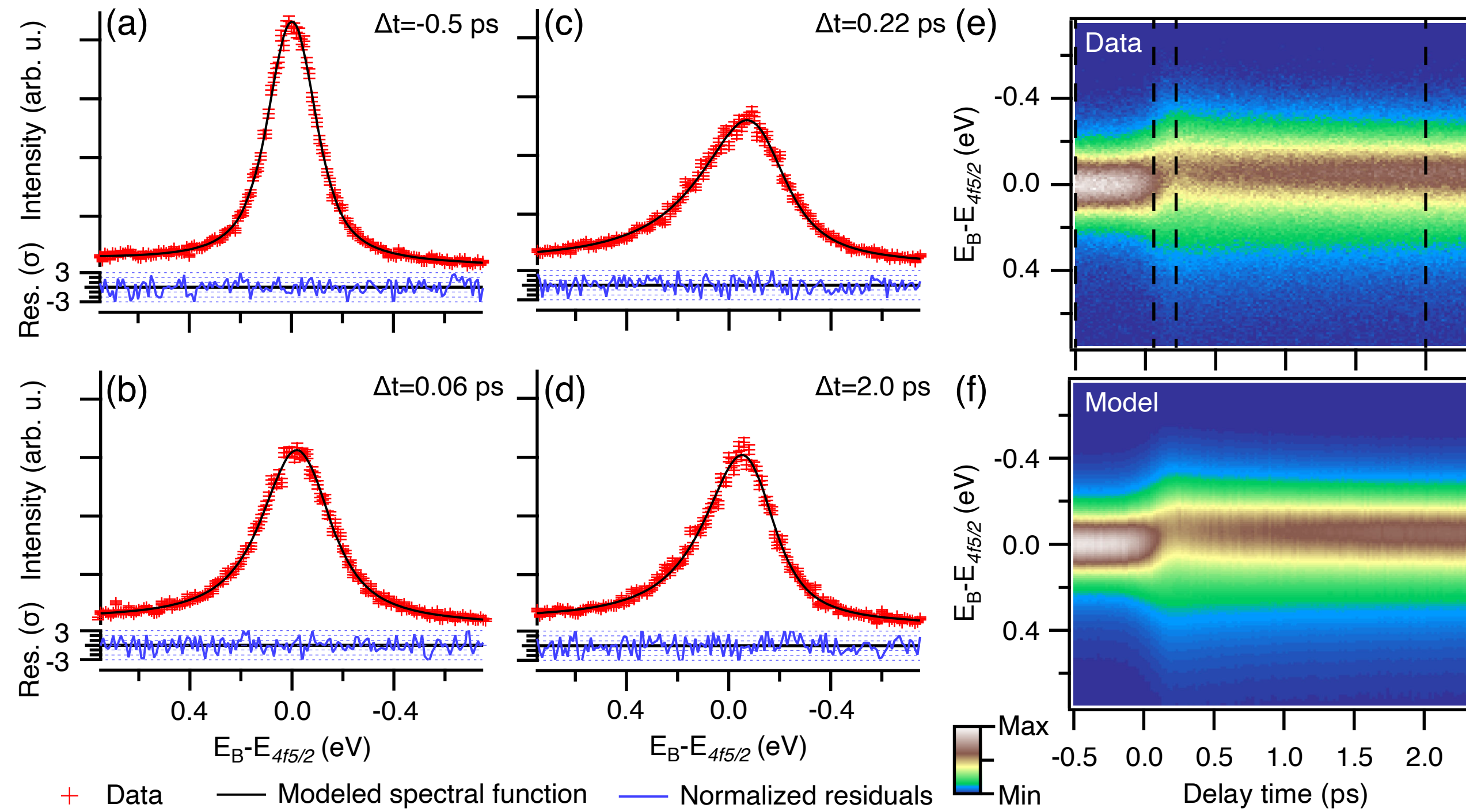
momentum microscopy @ FLASH



- much more efficient electron detection
- space charge issues



ultrafast XPS line shape analysis

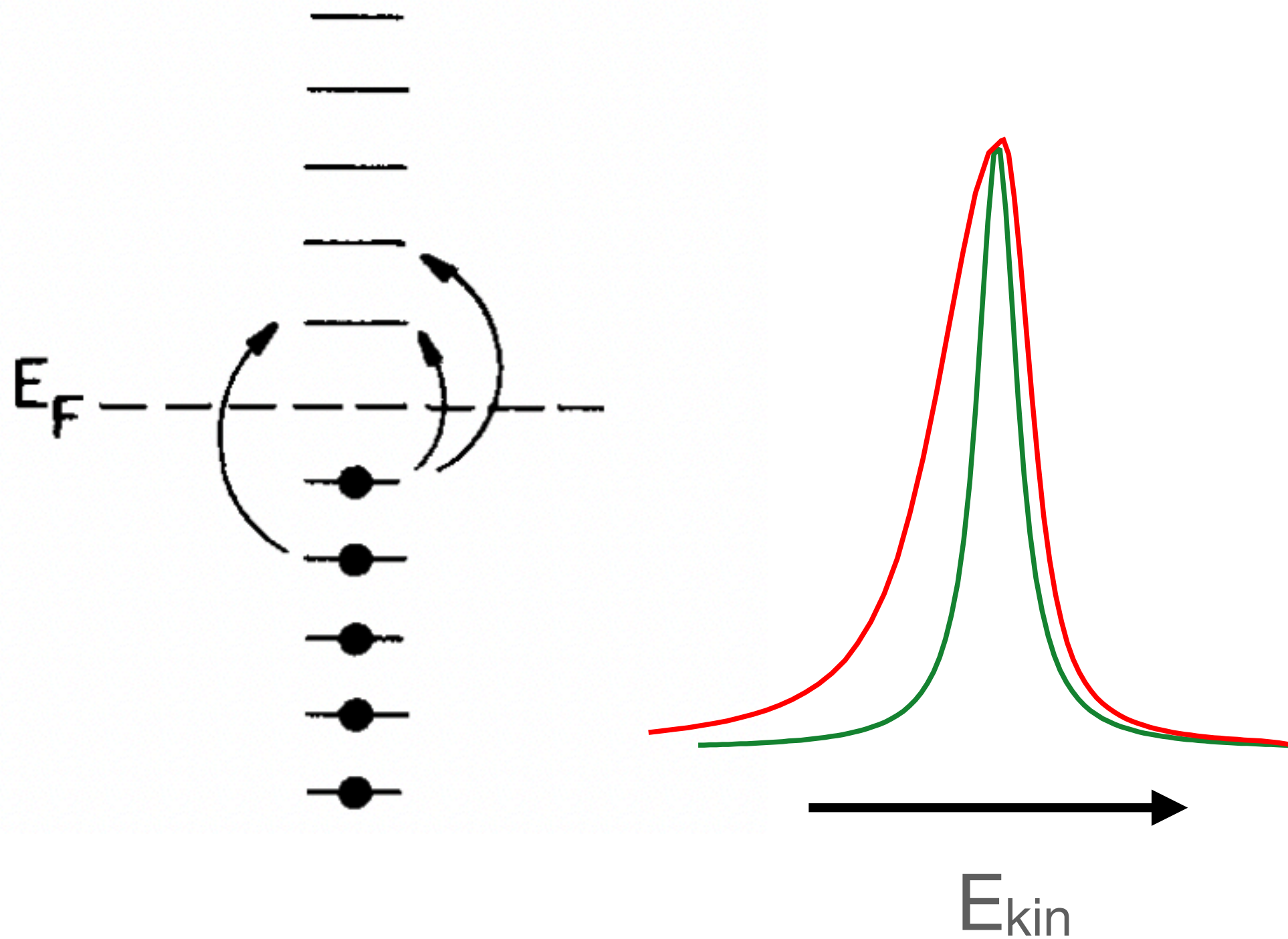




TEMPERATURE DEPENDENCE OF X-RAY PHOTOEMISSION SPECTRA:
FERMI-SEA RECOIL EFFECTS

S. Satpathy and John D. Dow

Department of Physics and Materials Research Laboratory
University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, U.S.A.

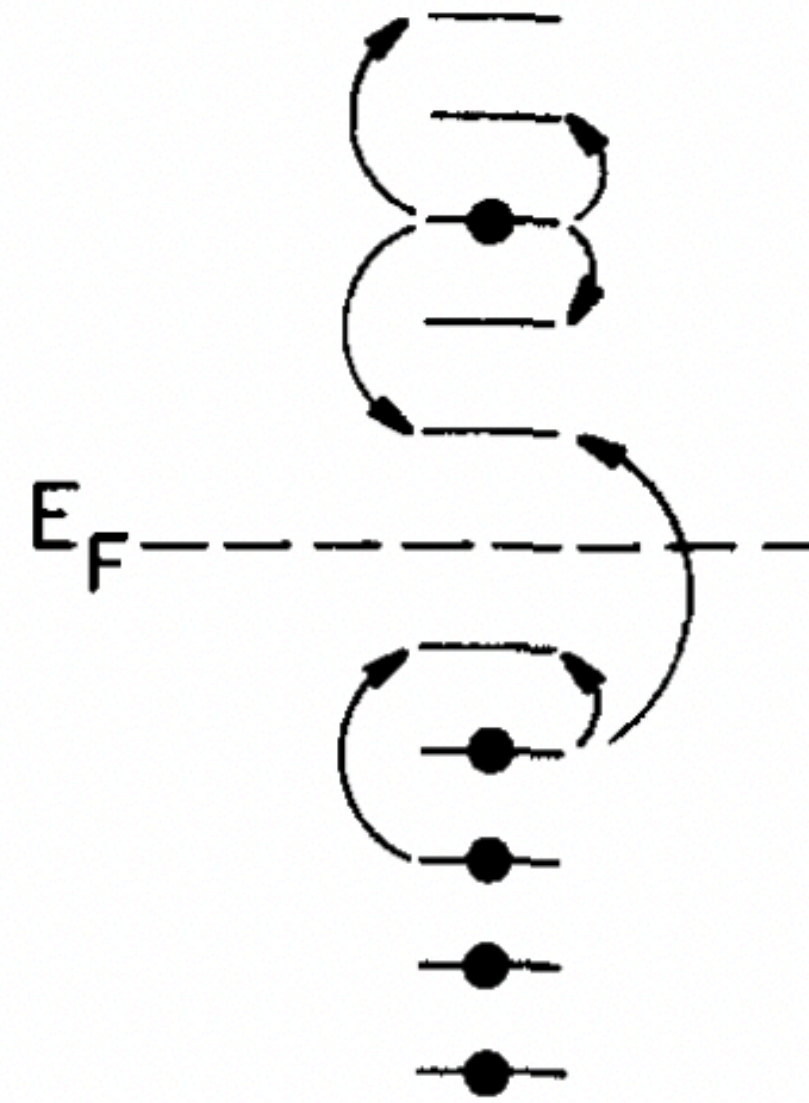
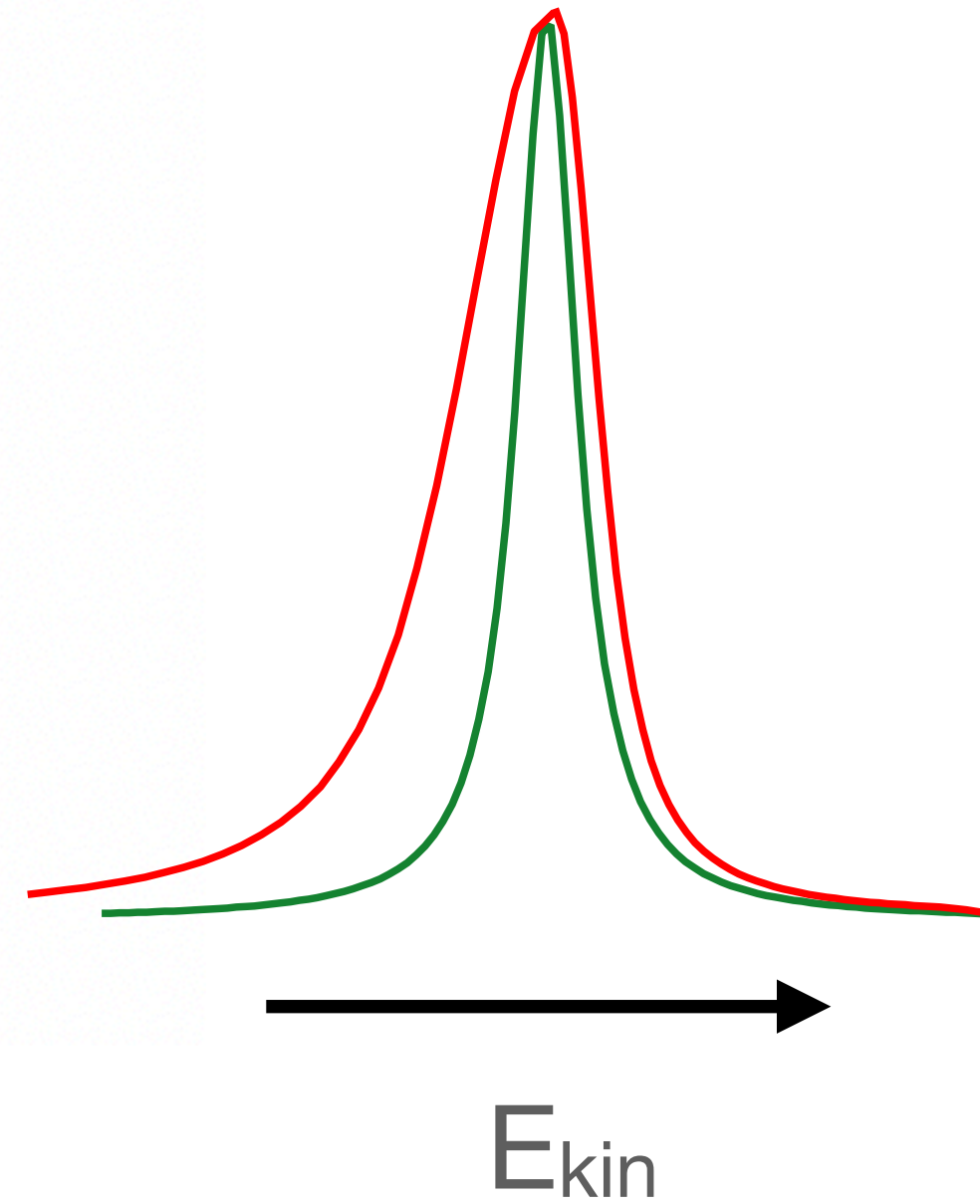
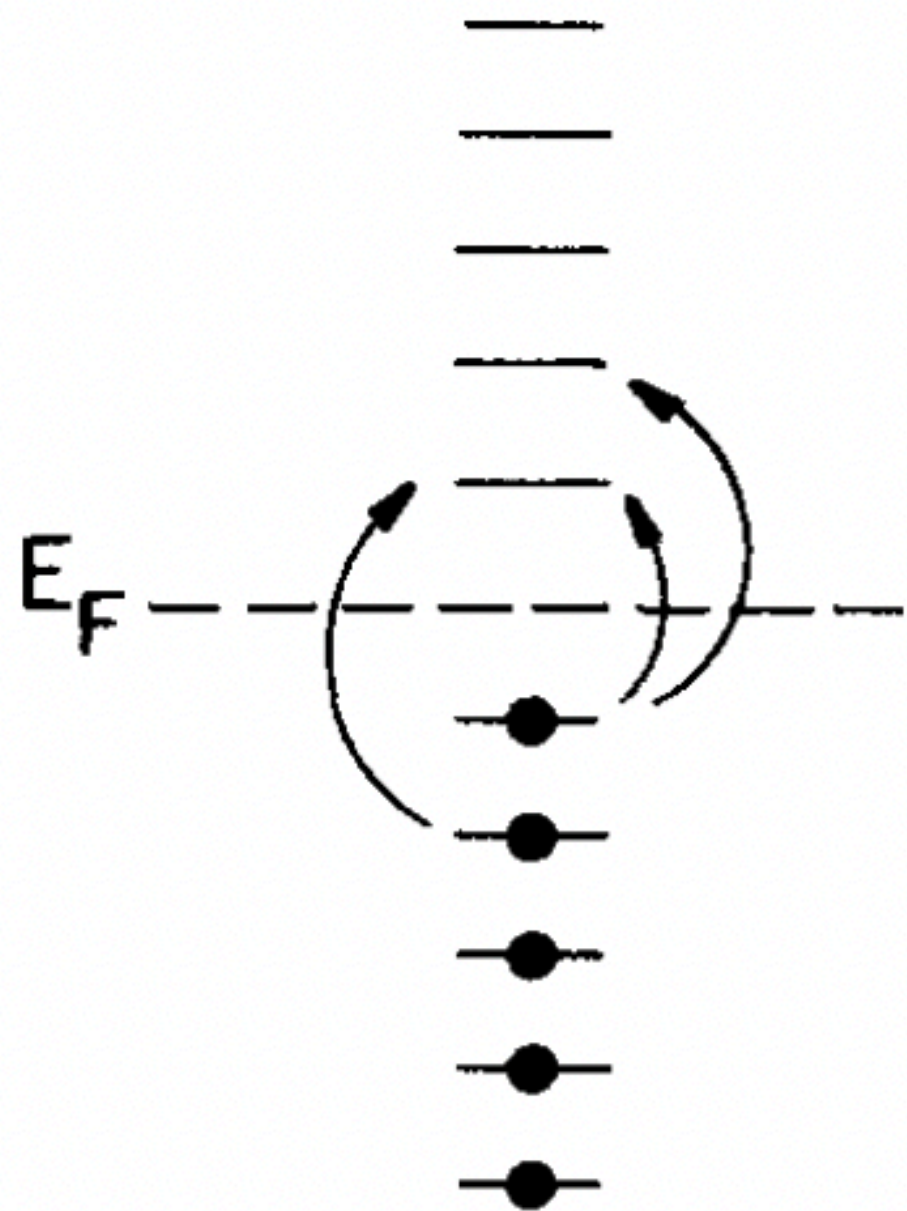




TEMPERATURE DEPENDENCE OF X-RAY PHOTOEMISSION SPECTRA:
FERMI-SEA RECOIL EFFECTS

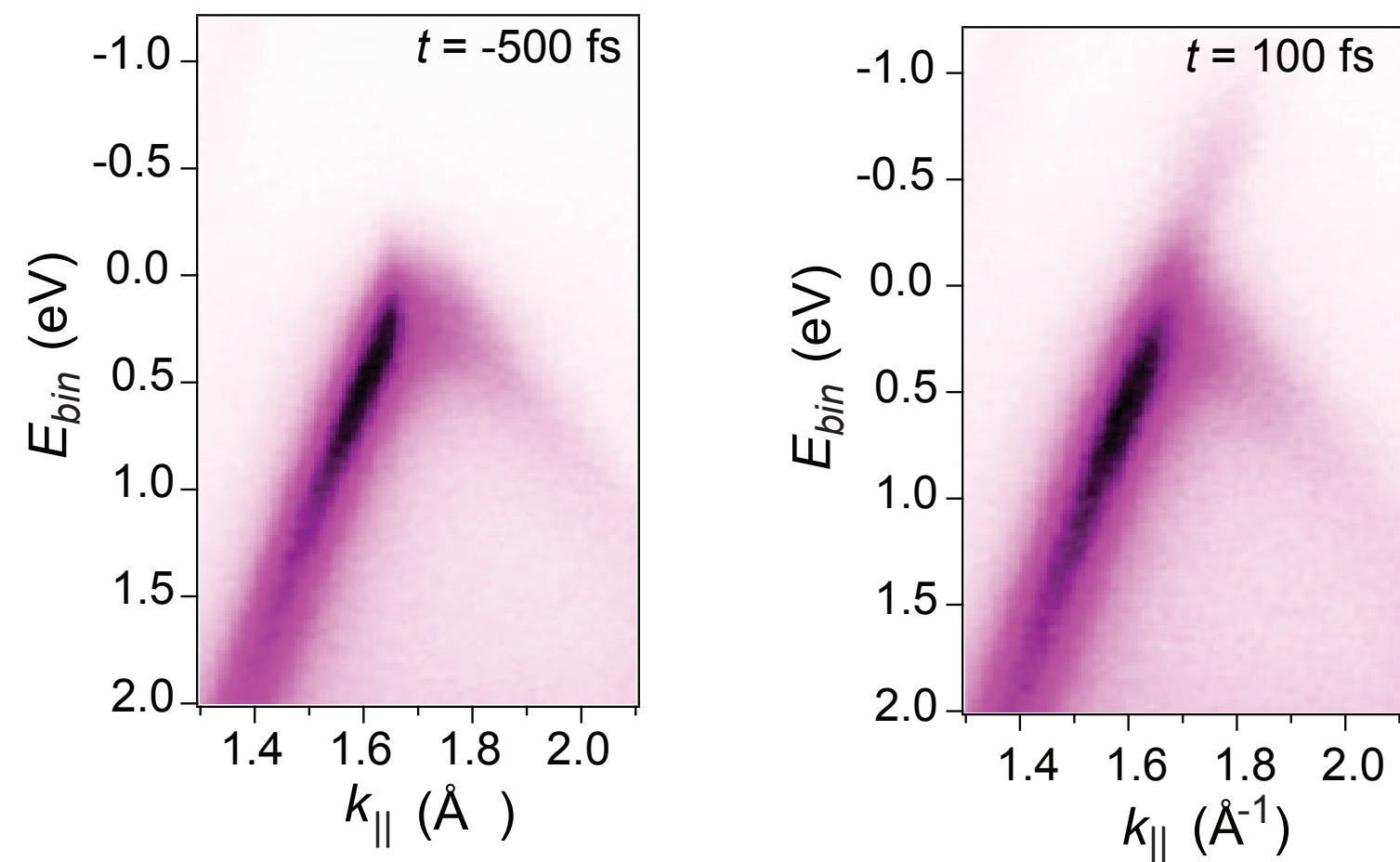
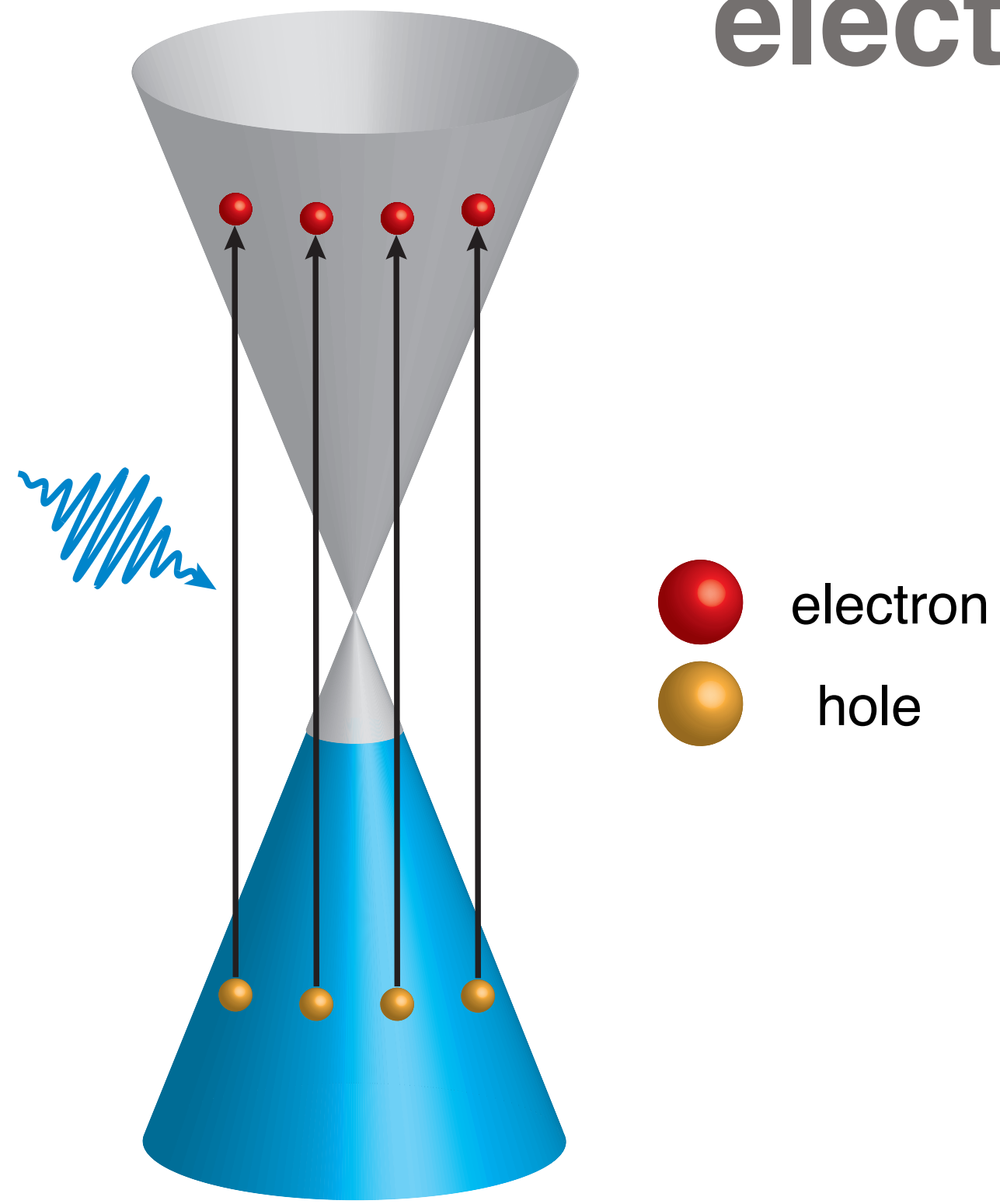
S. Satpathy and John D. Dow

Department of Physics and Materials Research Laboratory
University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, U.S.A.



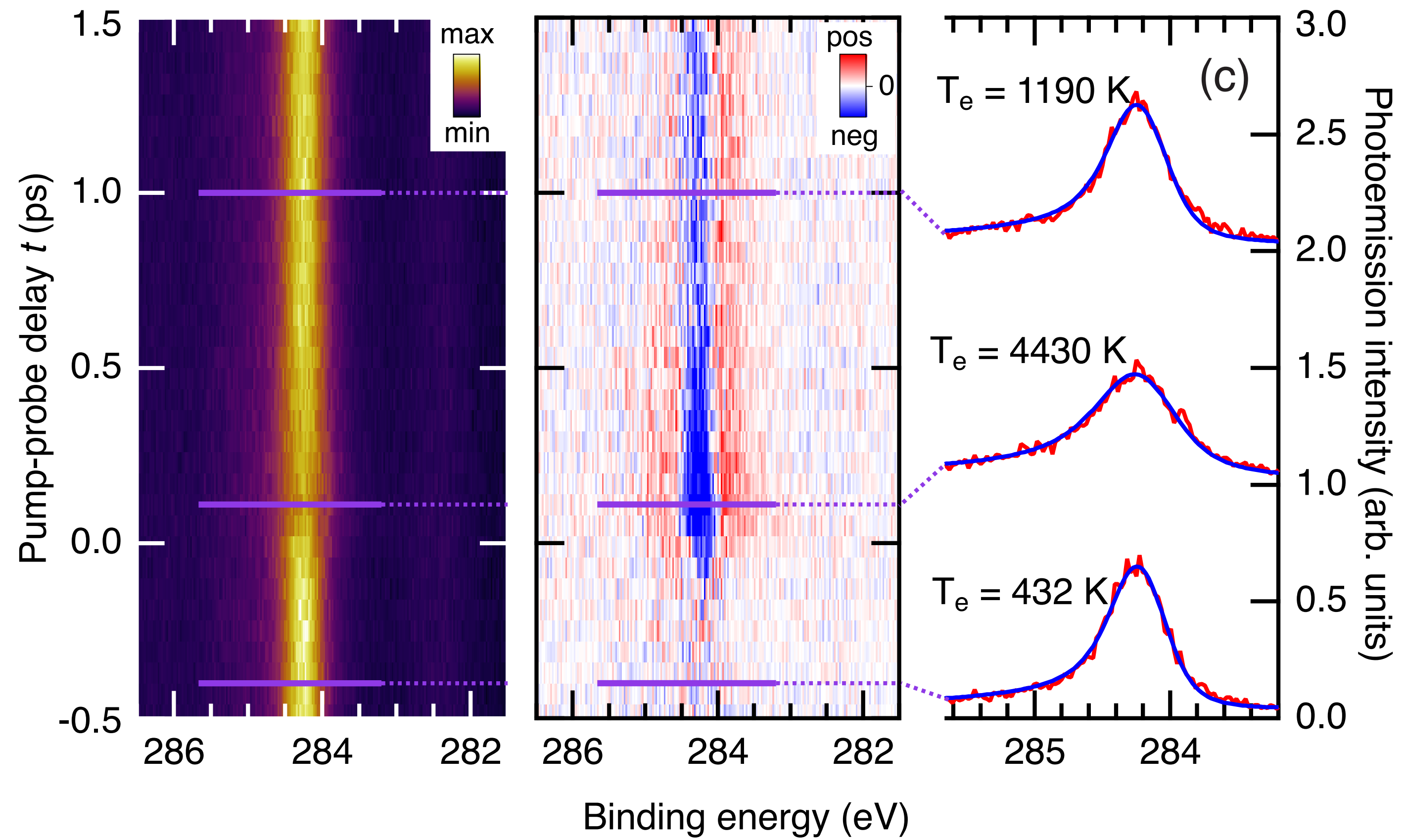
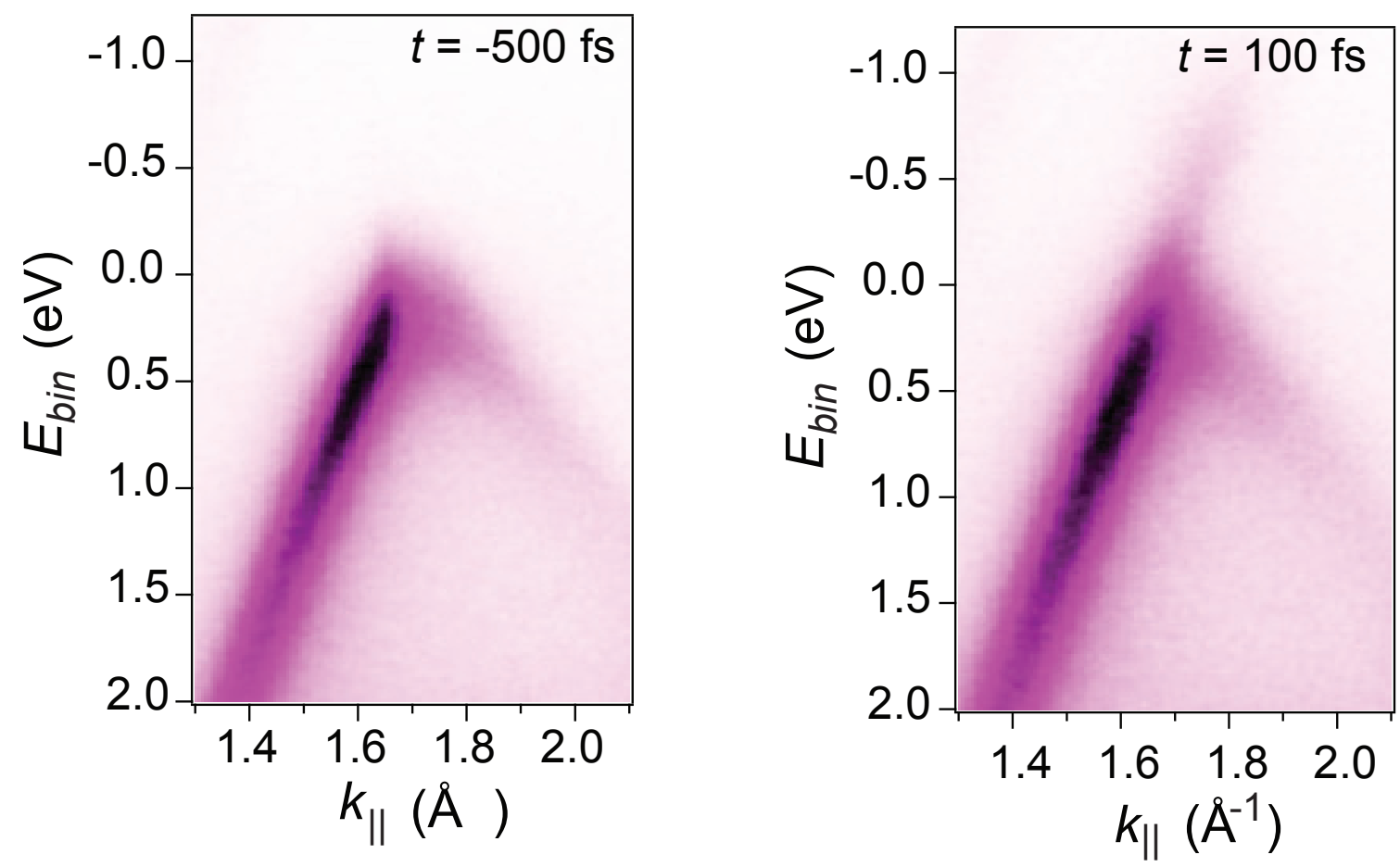
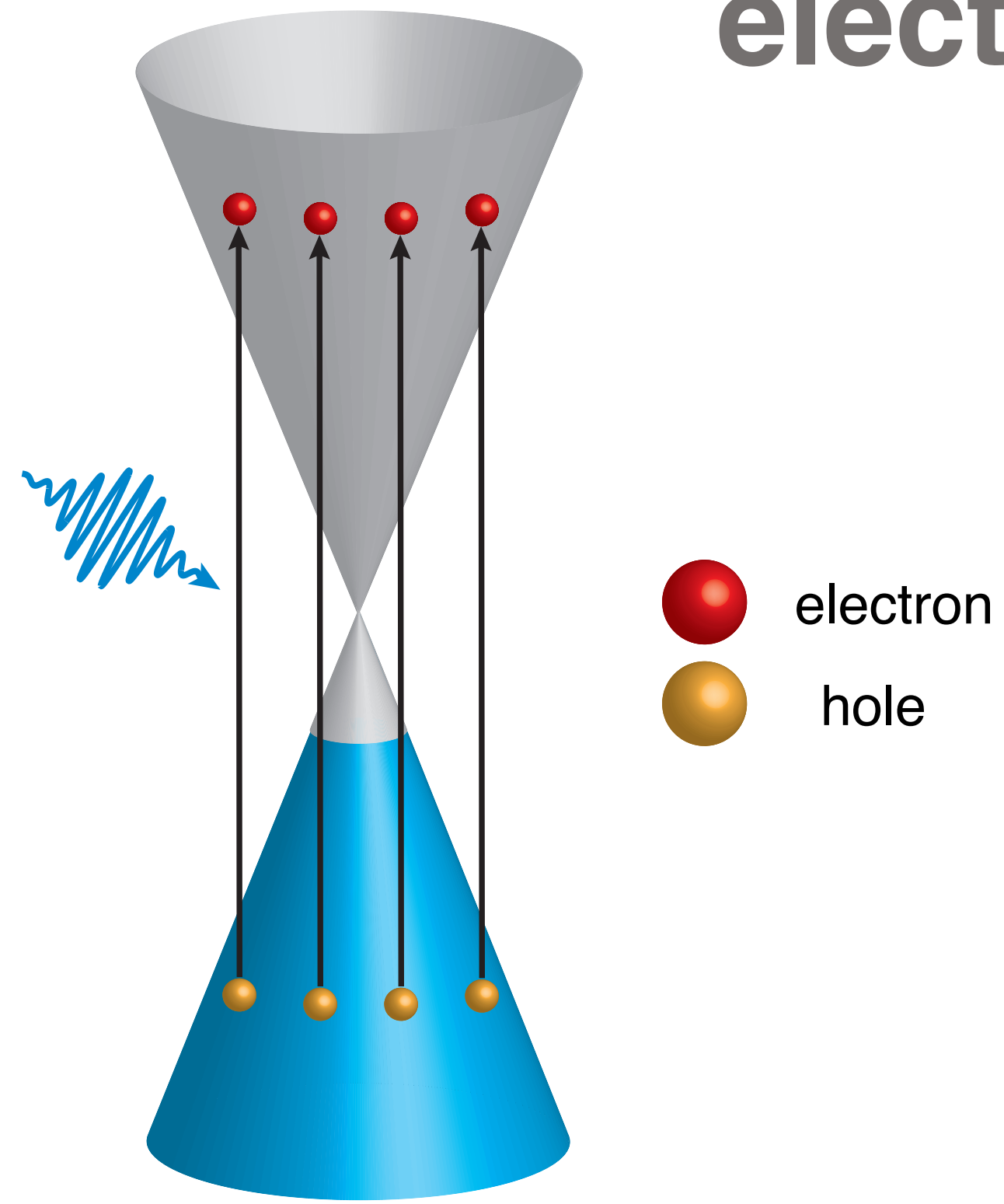


electronic temperature from XPS lineshape



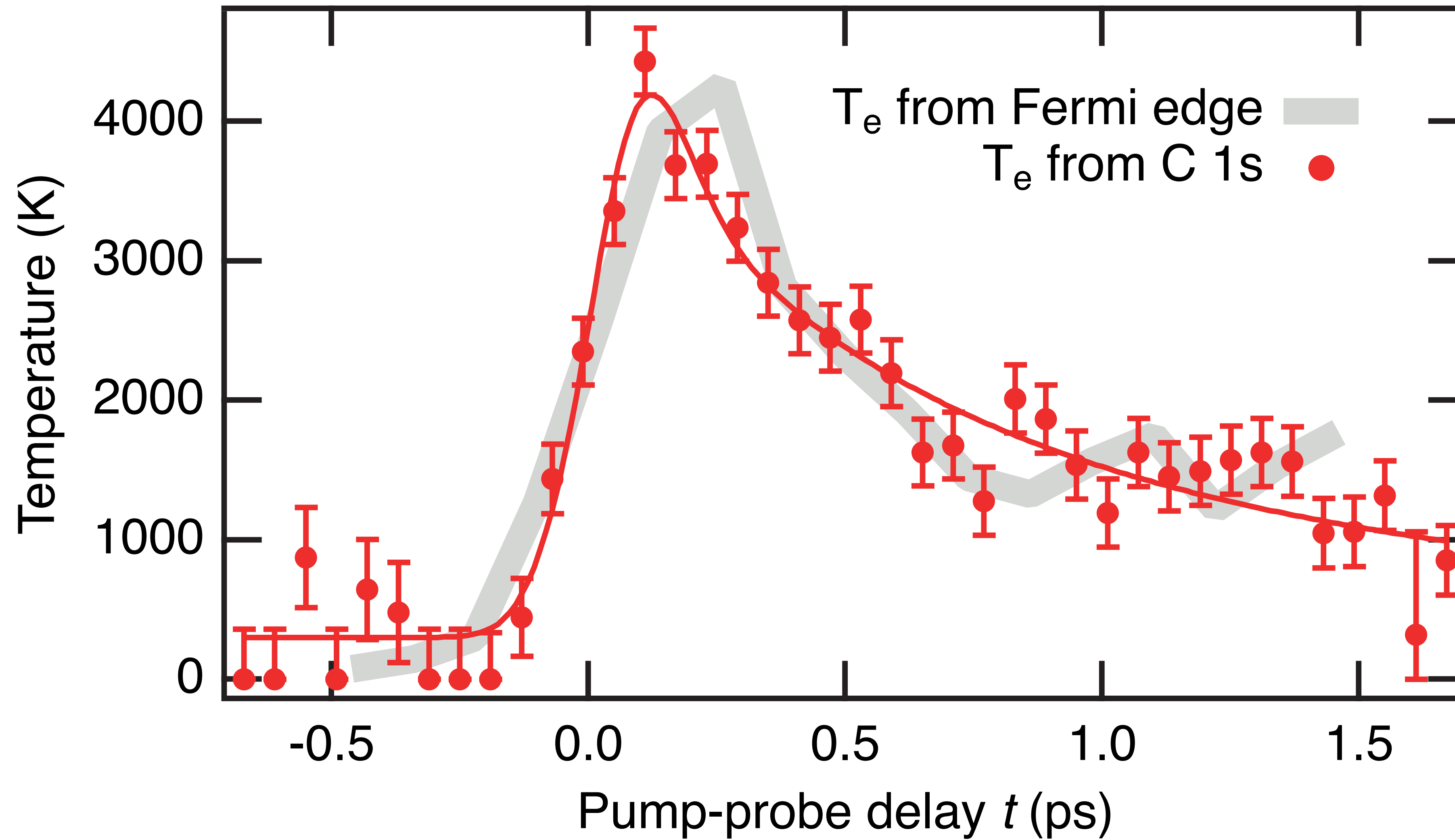


electronic temperature from XPS lineshape



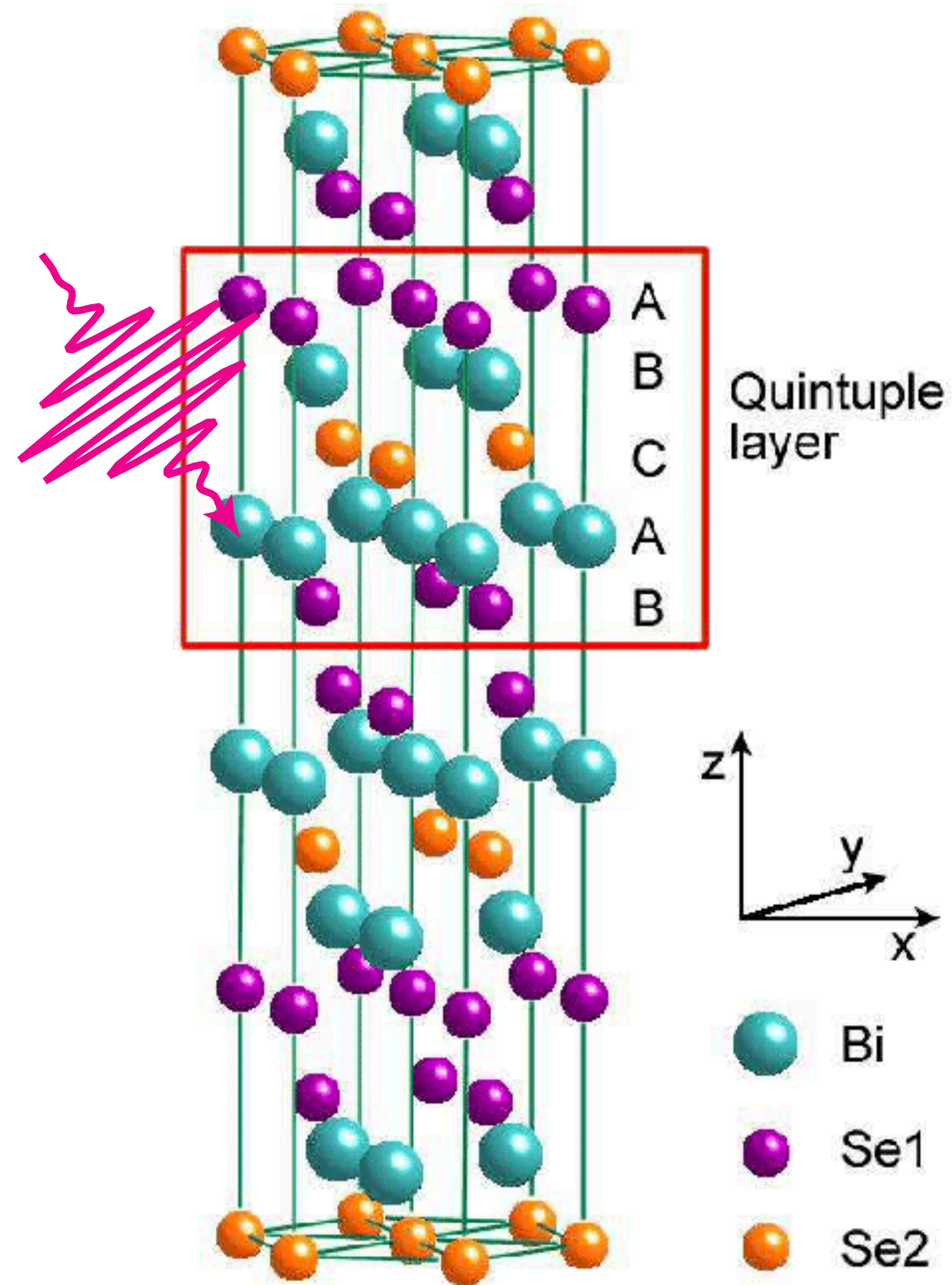


electronic temperature from XPS lineshape

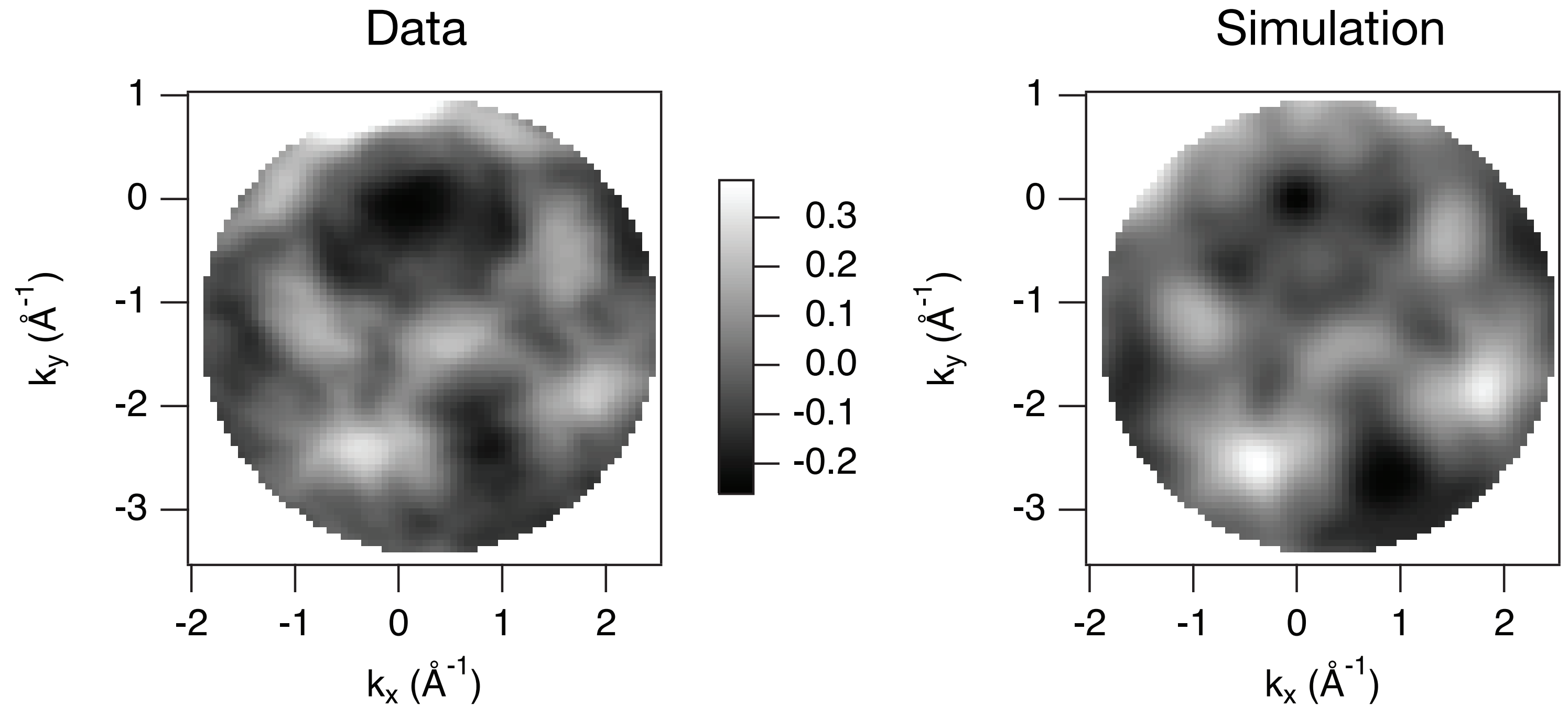




time-resolved XPD: coherent phonons in Bi_2Se_3



time-averaged data

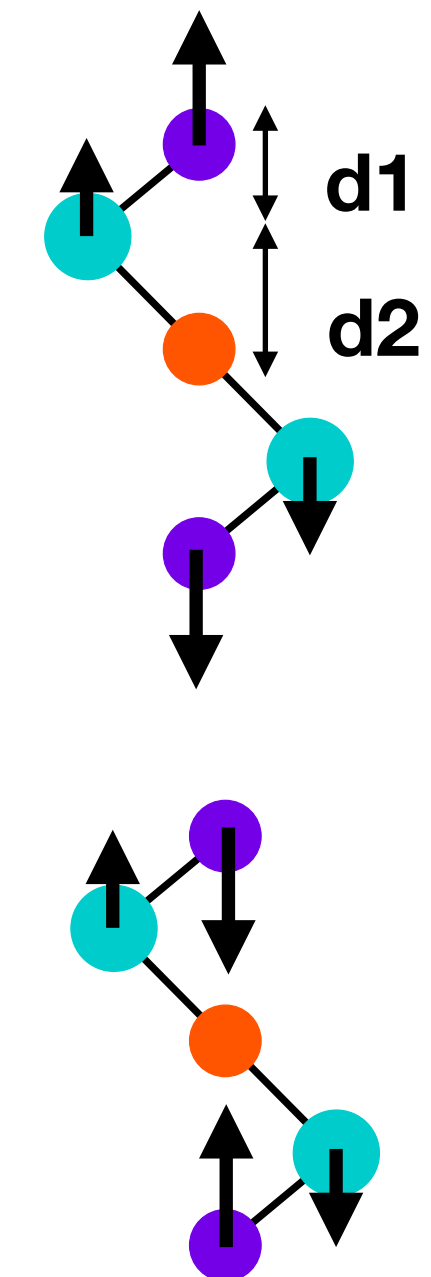
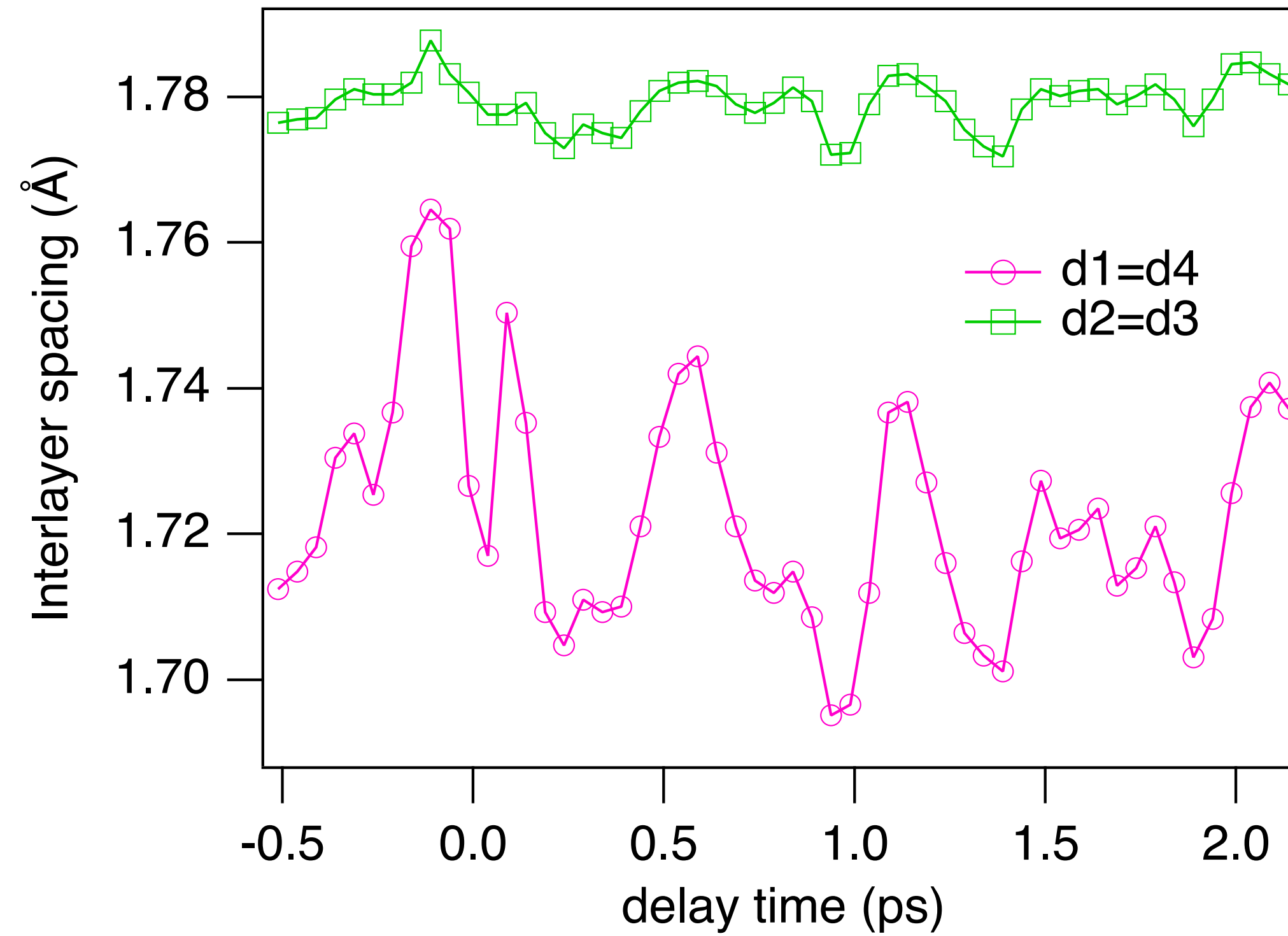




time-resolved XPD: coherent phonons in Bi_2Se_3

time-resolved structure (preliminary)

Change in interlayer spacing





conclusions

- promising initial experiments for time-resolved XPS and XPD with new and unexpected effects
- very challenging experiment in terms of achieving sufficient statistics
- space charge continues to be a real issue
- substantial gain at XFEL due to higher photon energy range



Aarhus University

Davide Curcio
Klara Volckaert
Paulina Majchrzak
Sahar Pakdel
Deepnarayan Biswas
Federico Andreatta
Sanjoy K. Mahatha
Marco Bianchi
Nicola Lanata
Jill A. Miwa
Søren Ulstrup
Philip Hofmann



ETH Zürich

Kevin Bühlmann
Rafael Gort
Yves Acremann



Central Laser Facility

Charlotte E. Sanders



FLASH, Desy

Dmytro Kutnyakhov
Michael Heber
Nils Wind
Federico Pressacco
Günter Brenner
Siarhei Dziarzhyski
Harald Redlin
Wilfried Wurth



Johannes Gutenberg University

Steinn Agustsson
Jure Demsar
Katerina Medjanik
Dmitry Vasilyev
Hans-Joachim Elmers
Gerd Schönhense



Kiel University

Florian Diekmann
Kai Rossnagel



Elettra Sincrotrone Trieste

Luca Bignardi
Daniel Lizzit
Paolo Lacovig
Silvano Lizzit



Chemnitz University of Technology

Florian Speck
Thomas Seyller



Forschungszentrum Jülich

Ying-Jiun Chen
Christian Tusche