



The Inelastic X-ray Scattering beam line ID20 at the ESRF

Ch. Sahle

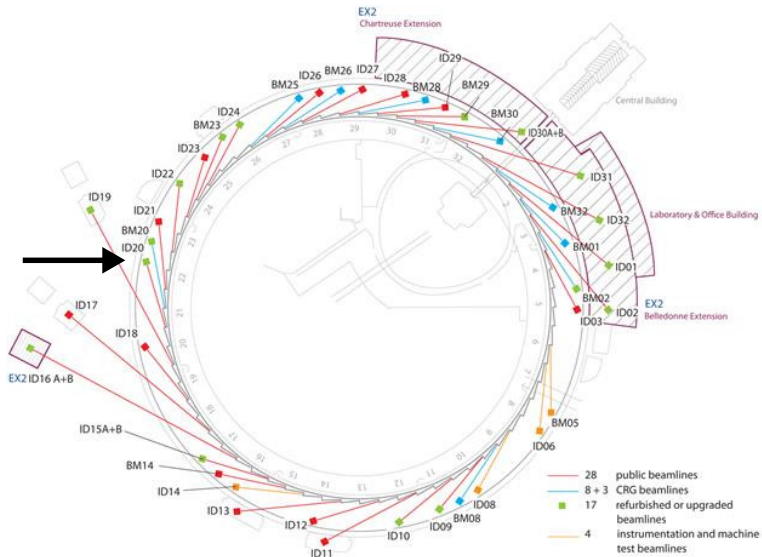
The European Synchrotron

June 26, 2019

ESRF, Grenoble, France



ID20

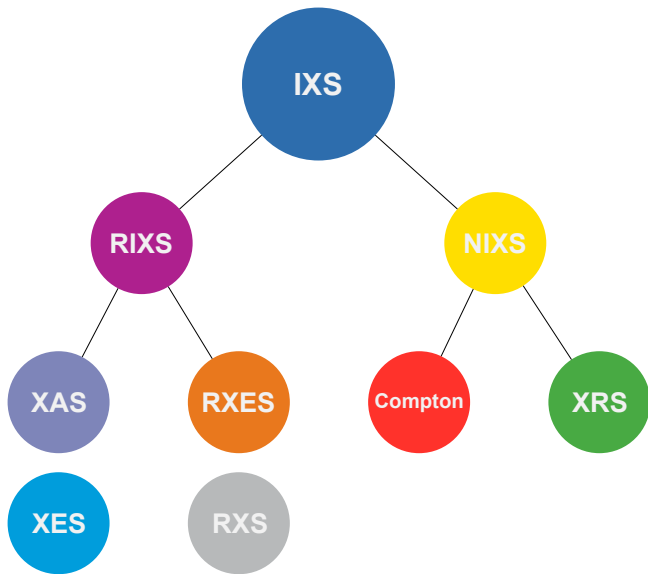


inelastic (hard) X-ray scattering

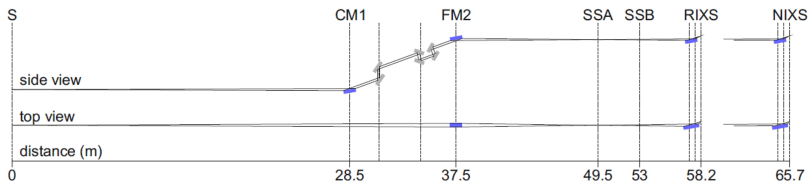
- ▶ photon in – photon out
- ▶ resonant and non-resonant IXS

$$\sigma = \frac{2\pi}{\hbar} \sum_f \left| \langle f | H' | g \rangle + \sum_n \frac{\langle f | H'' | n \rangle \langle n | H'' | g \rangle}{E_g - E_f} \right|^2 \times \delta(E_f - E_g + \hbar\omega)$$

techniques at ID20



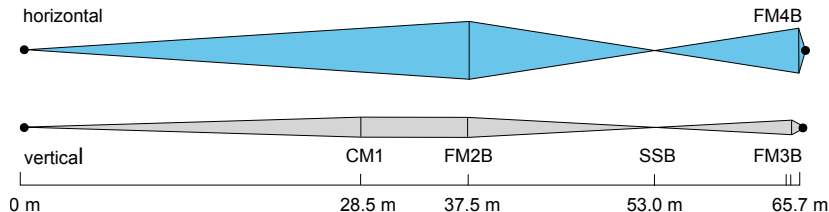
shared X-ray optics



- ▶ straightforward and stable design
- ▶ high flexibility (beam size, resolution, energy range)
- ▶ two spectrometers (high-resolution, large solid angle)

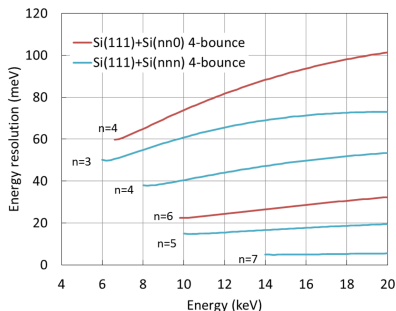
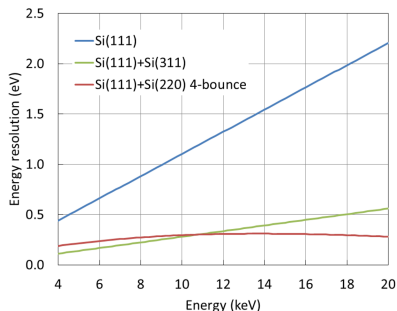
all credits to: G. Monaco, M. Krisch, M. Moretti Sala

focusing



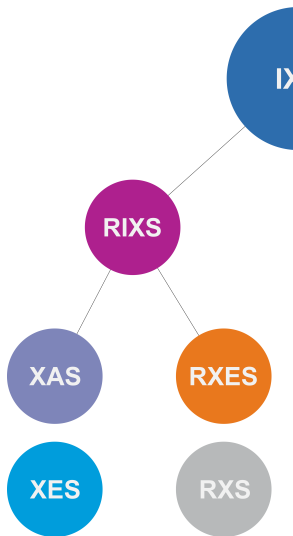
- ▶ CM1: maximize the throughput and energy resolution of the monochromator(s)
- ▶ FM2: create source image at secondary source (temporary experimental setups)
- ▶ KB (FM3, FM4): optimize the focal spot size at sample position

energy range and resolution



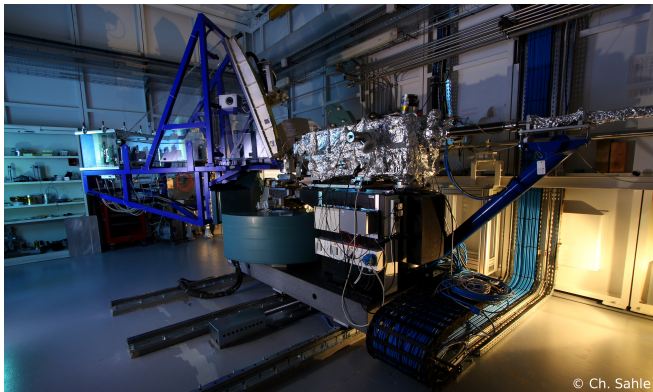
- ▶ Si(111) ($\Delta E/E \sim 10^{-4}$)
- ▶ Si(311) ($\Delta E/E \sim 10^{-5}$)
- ▶ Si(nnn), Si(nn0) 4-bounce
- ▶ Si(nnn), Si(844) back-scattering channel-cut ($\Delta E/E \sim 10^{-6}$ @ Ir L₃)

high-resolution IXS



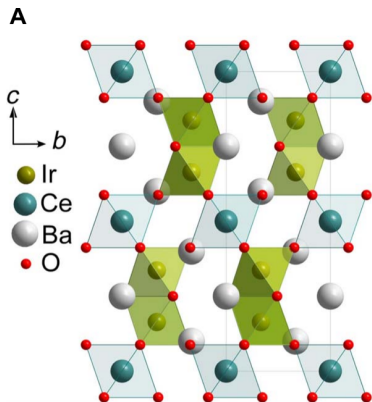
- ▶ energy/momentum resolution
- ▶ variable direction of q

high-resolution IXS



- ▶ 5 crystals in Johann-geometry
- ▶ 1m or 2m radius of curvature
- ▶ 0.025 - 2.0 eV resolution

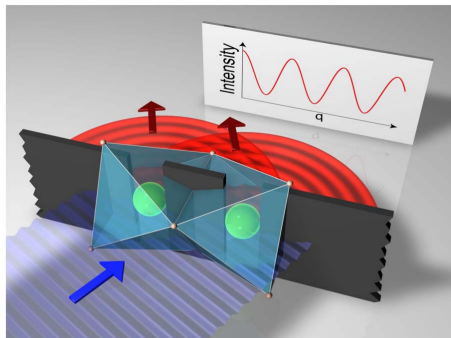
example - Young's double using Ir dimers



- ▶ insulating $\text{Ba}_3\text{CeIr}_2\text{O}_9$
- ▶ Ir - dimers (Ir^{4+})
- ▶ well localized core hole ($|n\rangle$)
- ▶ no "which-path" information ($|f\rangle$)

Revelli, A., M. Moretti Sala, G. Monaco, P. Becker, L. Bohatý, M. Hermanns, T. C. Koethe et al. "Resonant inelastic x-ray incarnation of Young's double-slit experiment." *Science Advances* 5, no. 1 (2019): eaav4020.

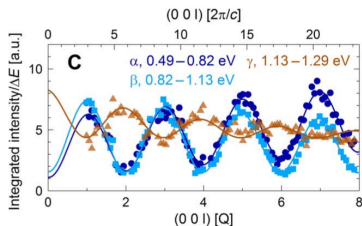
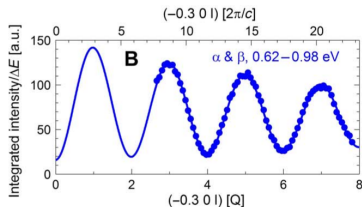
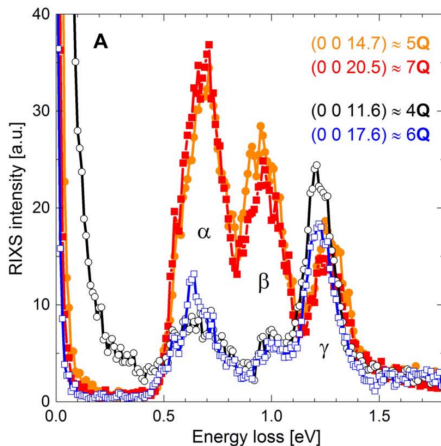
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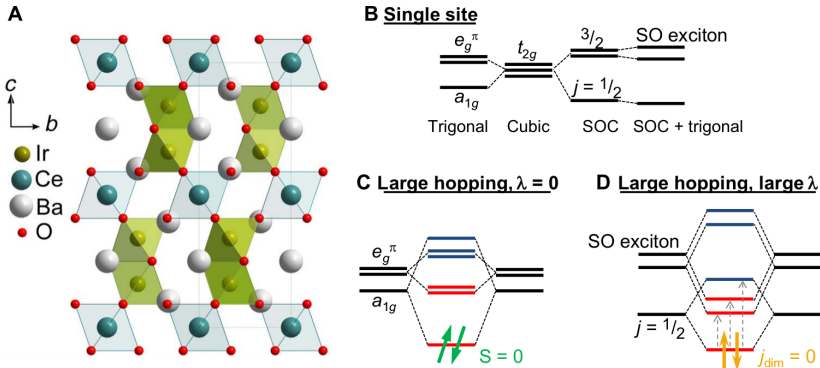
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RIXS - Young's double using Ir dimers



- ▶ $\alpha, \beta \sim \sin^2 \rightarrow$ bonding MO final state
- ▶ $\gamma \sim \cos^2 \rightarrow$ anti-bonding MO final state

RIXS - Young's double using Ir dimers



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RIXS interferometry

- ▶ inelastic incarnation of Young's double slit
- ▶ interference carries information about symmetry of excited states
- ▶ potential for materials containing dimers, trimers, heptamers, etc.

F. Gel'mukhanov, H. Ågren, Phys. Rev. A 49, 4378 (1994); Y. Ma, M. Blume, Rev. Sci. Instr. 66, 1543 (1995);

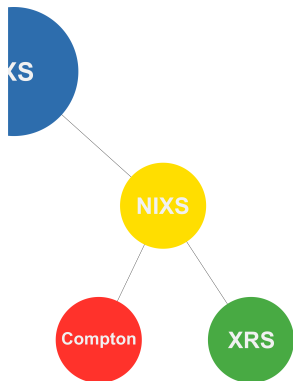
W. Schülke, C. Sternemann, Phys. Rev. B 84, 085143 (2011); Revelli, A., M. Moretti Sala, G. Monaco, P. Becker,

L. Bohatý, M. Hermanns, T. C. Koethe et al. "Resonant inelastic x-ray incarnation of Young's double-slit

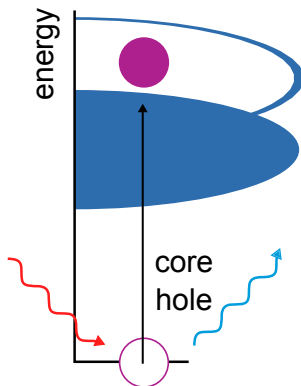
experiment." Science Advances 5, no. 1 (2019): eaav4020.

NIXS

- ▶ energy resolution/flux
- ▶ large solid angle
- ▶ fixed analyzer Bragg angle
- ▶ q-resolution

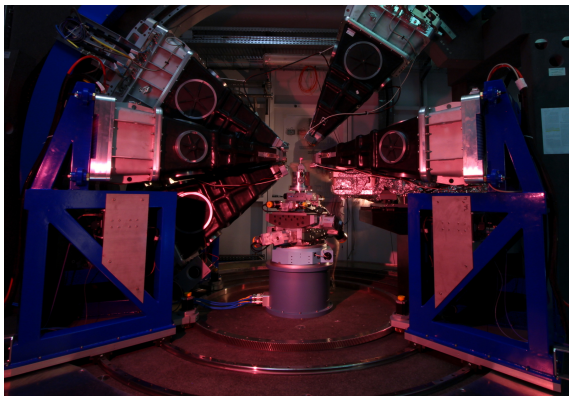


XRS - photon energy loss spectroscopy

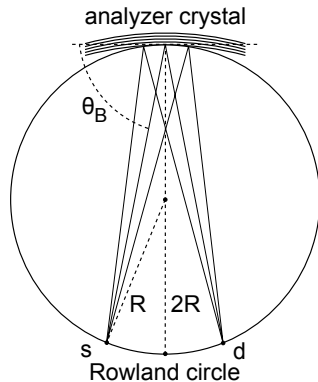


- core-hole through energy loss

NIXS

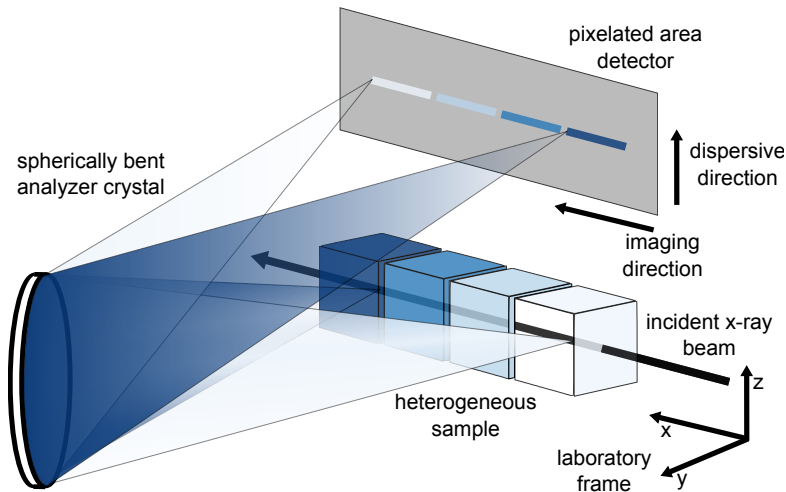


- ▶ 72 spherically bent Johann crystals
- ▶ mediocre energy resolution (0.7 eV at Si(660))
- ▶ low background (vacuum chambers, collimators)



- point-to-point focus
- 72 individual Rowland circles

DT - X-ray imaging with chemical bond contrast

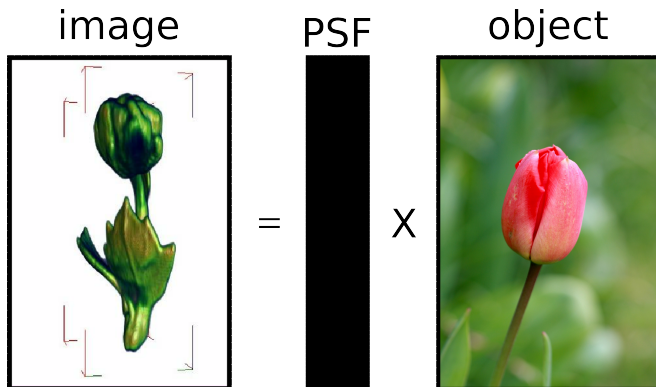


multi analyzer DT imaging

$$\mathbf{D}_a(\omega, y, z) = I_0 \int \mathbf{P}_a(x) t_{x,y,z}^a(\omega_1 - \omega) t_{source}^{x,y,z}(\omega_1) \sum_c \rho_c(x, y, z) e_c(\omega, q_a) dx$$

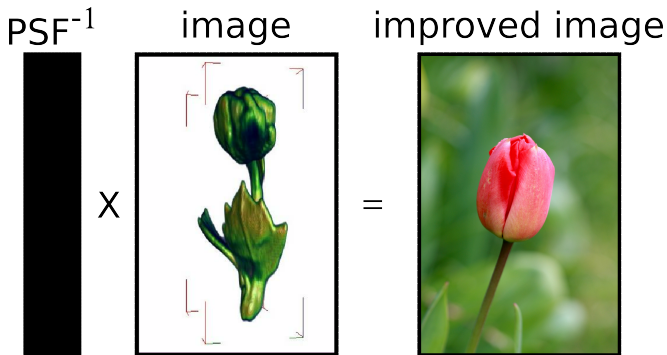
Sahle, Ch J., A. Mirone, T. Vincent, A. Kallonen, and S. Huotari. "Improving the spatial and statistical accuracy in X-ray Raman scattering based direct tomography." J. Synchrotron Rad. 24, no. 2 (2017): 476-481.

multi analyzer DT imaging



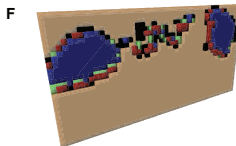
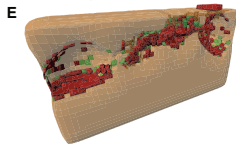
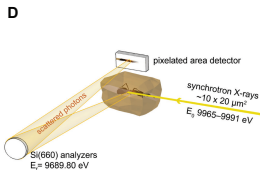
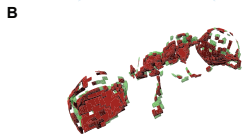
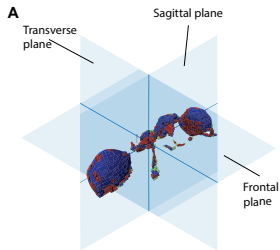
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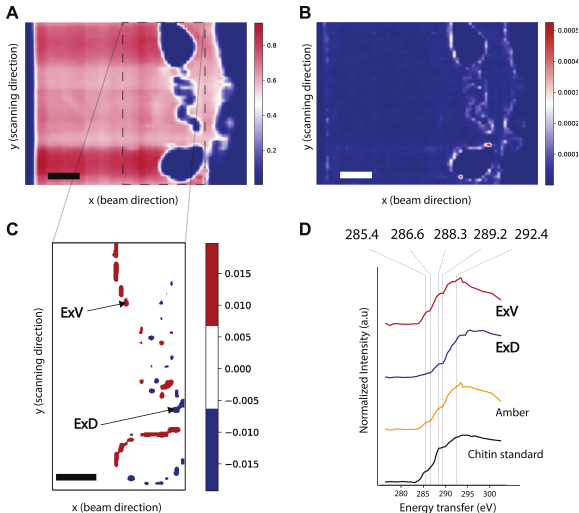
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Carbon speciation in organic fossils



- ▶ 53 Mya old amber
- ▶ 50 μm^3 voxel
- ▶ 0.5 eV step size
- ▶ C K-edge
- ▶ ca. 12 h

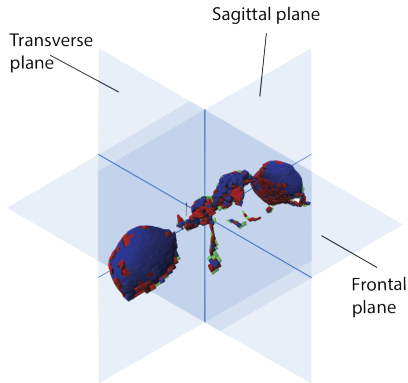
Carbon speciation in organic fossils



- a) total intensity in virtual cross section
- b) quadratic errors of linear combination fit
- c) chitin distribution
- d) extracted spectra

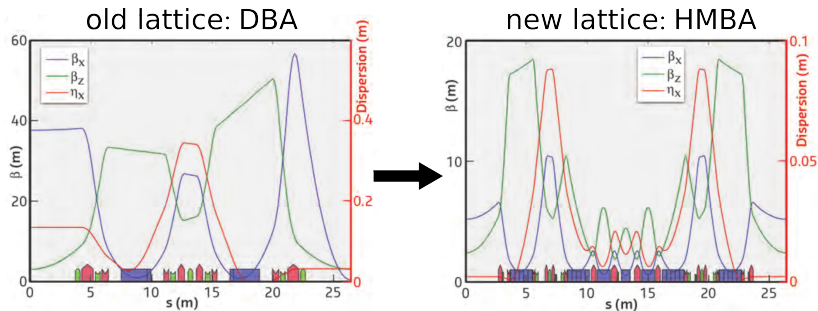


Carbon speciation in organic fossils



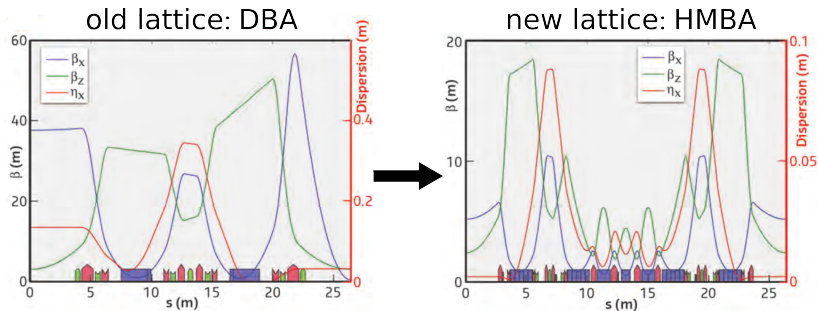
- ▶ low-Z chemistry in 3D
- ▶ non-invasive
- ▶ not yet non-destructive

EBS - extremely bright source



- ▶ 7-bend achromat with longitudinal gradient
- ▶ horizontal emittance reduced by factor ≥ 30
- ▶ same beta function at each insertion device
- ▶ decreased energy loss per turn

EBS - extremely bright source



- ▶ machine commissioning starts December 2019
- ▶ BL commissioning starts March 2020
- ▶ user operation back in August 2020

EBS - extremely bright source

- direct consequences for ID20's source ($4\times$ U26 undulator)

10 keV	source size [$\mu\text{m rms}$]		source divergence [$\mu\text{rad rms}$]	
	H	V	H	V
old lattice	411.6	6.2	11.5	5.1
new lattice	28.2	6.1	7.2	5.1

EBS - extremely bright source

- direct consequences for ID20's x-ray spot size

spot size at sample position	EH2 [$\mu\text{m rms}$]		EH3 [$\mu\text{m rms}$]	
	H	V	H	V
old lattice	20	7	18	6
new lattice (current KB)	4	7	4	6
new lattice (modified KB)	4	4	4	4

Thank you

- ▶ **K. Gilmore** of BNL (former ESRF), Brookhaven
- ▶ **R. Georgiou, P. Gueriau, L. Bertrand** of IPANEMA, Paris
- ▶ **J.-P. Rueff** of Soleil, Paris
- ▶ **U. Bergmann** of SLAC, Palo-Alto
- ▶ **M. Moretti Sala** of Politec. Milano (former ESRF)
- ▶ **A. Revelli, M. Güninger** of Uni Köln, Köln