Parameters Discussion

11th December 2018, ALBA, Barcelona

Jim Clarke, STFC Daresbury Laboratory

WP2 FEL Science Requirements and Facility Design

- **Task 2.1 -** FEL user scientists and potential users will provide specification for the Hard X-ray FEL output parameters (in terms of wavelength range, pulse energy, polarisation, beam structure, pulse duration, synchronisation to external laser, etc.).

- **Deliverable 2.1** - A report summarising the requests from the users and defining the performance specifications for the FEL, **(31/12/18).**

- **Task Leader – Vitaliy Goryashko, Uppsala University**
  - **Vitaliy will provide a report from the User Meeting that was held in November**

- **Agreeing the FEL specification this week is a key outcome from this meeting**

REMINDER: Compact Light FEL Preliminary Specification

Two informal meetings were held with leading proposers of UK XFEL

- All of them are experienced users of LCLS, and other FEL user facilities, including European XFEL now
- CompactLight proposal stated that “we will develop a hard X-ray FEL design tailored to the UK user specifications”

General comments from UK users

- **If UK XFEL is not world leading then why would anyone want to use it?**
- **We will all just go to the best facility for our research whatever country it is in**
- **We can’t justify funding UK XFEL unless it has unique capabilities, enabling science that is not possible on other FELs**

- A preliminary set of parameters were discussed in Trieste based on this input

REMINDER: CompactLight Preliminary Specification Notes

250 eV – to cover the carbon K edge

25 keV – requested by group studying extreme materials

Pulse duration – 100as isolated pulses have definite science need identified (atomic and molecular physics), *case for shorter pulses than 100as to be determined*

Pulse duration – 50 fs not a definite requirement, *just a typical number*

Pulse energy – 1mJ at 25keV highly desired by extreme materials, *higher welcome* but may not be realistic

Repetition rate – 100Hz at 25keV (high power lasers are combined in experiment and they only have low repetiton rate)

Repetition rate – 1000Hz or greater *highly desirable* for the soft X-ray, 250eV to 2keV

Two colour output is required – see slide

Two pulse output required with time separation of pulses set by the FEL between -20fs and +40fs. Larger time separations will be achieved within the beamline (split and delay)

Polarization – variable, selectable below 2 keV.

Polarization – above 2keV *to be determined.*

We are not expected to cover this photon range with one beamline

There is a natural beamline breakpoint at ~2keV where gratings are replaced by crystals

REMINDER: CompactLight Preliminary Specification

The table below separates the FEL output requirements into the two regimes of operation (soft/hard x-ray) to show which parameters are required in combination.

	Soft x-ray	Hard x-ray
Photon energy [keV] (min-max)	0.25 - 2	2 - 25
Wavelength [nm] (max-min)	5 - 0.6	0.6 - 0.05
Repetition rate [Hz]	1000	100
Maximum pulse energy [mJ]	Not specified	1 (at 25 keV, less at other energies?)
Number of photons	Not specified	2.5 x 10^{11} at 25 keV
Pulse duration [fs]	0.1 – 50	
Polarisation	Variable, selectable	Not specified
Two-colour pulses: time separation [fs]	-20 -> +40	
Two-colour pulses: photon energy variation (max. of E2/E1)	2 (270-530eV), 1.2 for the rest of the range	1.1

REMINDER: CompactLight Preliminary Specification Proposal

	LCLS	SACLA	PSI ARAMIS	LCLS-II HXR	PAL XFEL HXR	EUXFEL HXR	CompactLight
Min Photon Energy (keV)	0.27	5	1.8	1.03	2.06	3.1	0.25
Max Photon Energy (keV)	12.4	15.5	12.4	25	20.6	25	25
Max Pulse Energy (uJ)	6000	250	150				1000
Pulse Duration (fs)	2 - 100	20 - 30	20				0.1 - 50
Pulses/s	120	60	100	120	60	27000	100 to 1000
Beam Energy (GeV)	15	8.5	5.8	15	10	17.5	TBD

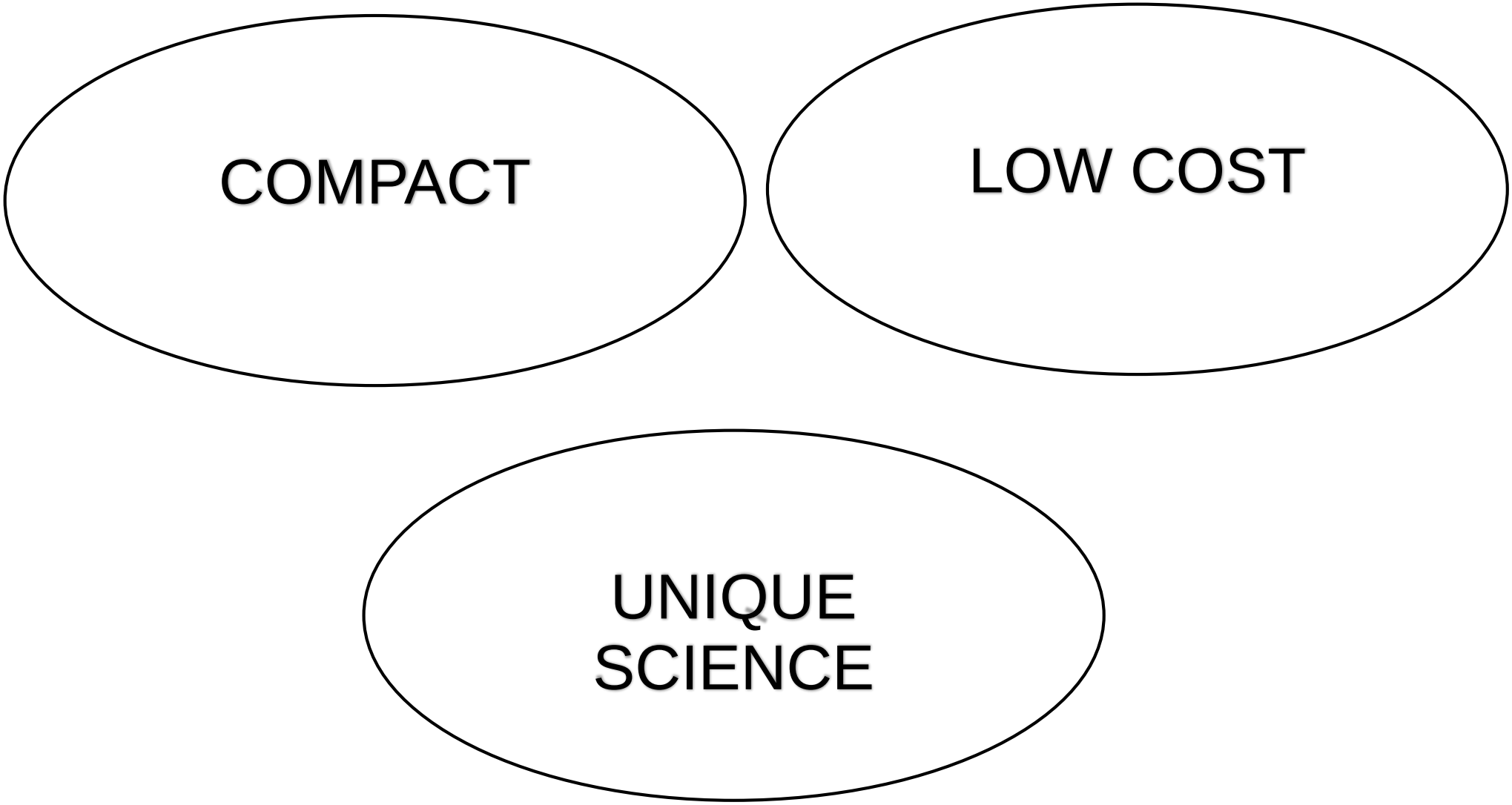
IOP Publishing Reports on Progress in Physics
Rep. Prog. Phys. 80 (2017) 115901 (73pp) https://doi.org/10.1088/1361-6633/aa7cca

Review

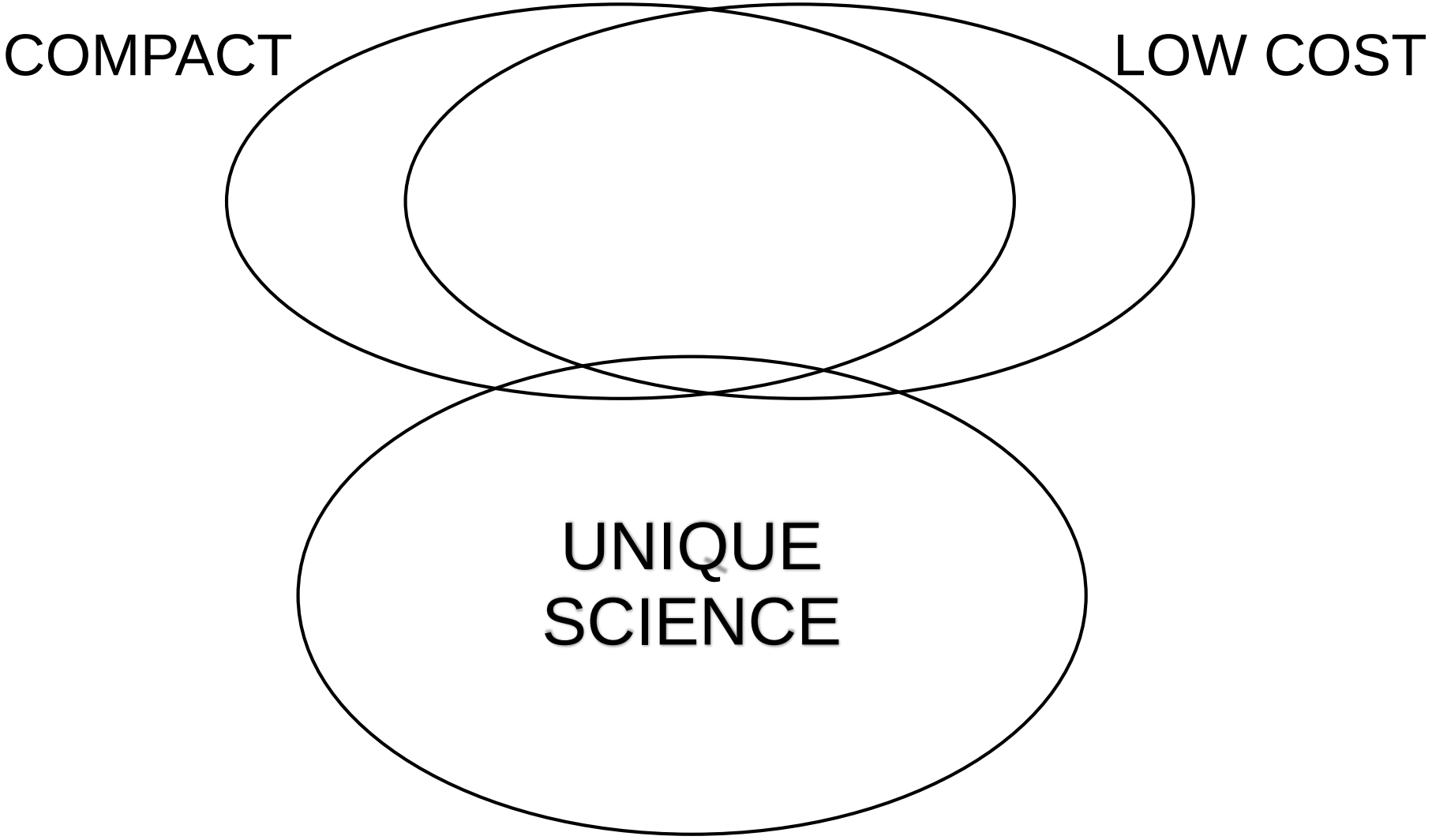
Short-wavelength free-electron laser sources and science: a review*

E A Seddon[1,2,3], J A Clarke[1,3], D J Dunning[1,3], C Masciovecchio[4], C J Milne[5], F Parmigiani[4,6,7], D Rugg[8], J C H Spence[9], N R Thompson[1,3], K Ueda[10], S M Vinko[11], J S Wark[11] and W Wurth[12]

What is our over-arching motivation?



Compatibility?



Key Messages from Users – Consistent across all research disciplines

- Stability
- Peak Brightness
- Synchronisation
- Polarization
- Repetition Rate
- Full Coherence
- Two pulses
- Two colours

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Compatible with Compact solutions?

Less Compatible with Compact solutions?

The Highest Photon Energy Drives the Electron Beam Energy: 3 Options

- **25 keV**
  - High Energy Density Science, Matter in Extreme Conditions (e.g. planets, stars)
  - Small niche community?
  - Dedicated end station on Euro-XFEL
  - Nothing special about “25” – higher the better
- **16 keV**
  - Suggested by Life Scientists for Serial Femtosecond Crystallography (SFX)
  - Also on Euro-XFEL (very high rep rate) but ~100Hz facilities well suited to fixed target delivery experiments which can be very competitive
  - Picked out as good alternative to liquid jets
  - Large and rich community
- **12.4 keV**
  - Standard FEL – satisfies many users

Alternate sample delivery method(s)

Fixed target sample delivery has many advantages

setup M. Sikorski, et al, SPB/SFX

Jet, B. Doak & R. Shoeman, Max Planck institute for Medical Research (with XFEL sample environment)

Aerosol Jet, Uppsala University with XFEL sample environment

Photon Beam Parameters for future (TR-) SFX Experiments

	Present	Future Liquid jet experiments	Future Fixed target experiments
Repetition rate	Up to MHz rates	MHz rates possible and in many cases desirable	Presently ~120 Hz, and perhaps up to low kHz possible
Pulse energy	Few mJ	At least few mJ	At least few mJ
Photon energies	5-16 keV	5-16 keV (Some case for even higher energies, if suitable detector exists)	5-16 keV (Some case for even higher energies, if suitable detector exists)
Pulse duration	Tens of fs	Perhaps shorter than tens fs	Perhaps shorter than tens fs
Bandwidth	~0.5%	Ideally variable up to few %	Ideally variable up to few %

- **Fixed target sample delivery** is limited to perhaps **low kHz rates**, however, is also a very viable way of doing structural biology at XFELs
- Also yes much less sample (which can often be very valuable)

Funded by the
European Union

Compact

indexed images **25,000**

hit ratio = 5%		image rate	time to collect full SFX dataset			
facility	detector	Hz	seconds	minutes	hours	days
LCLS	CSPAD	120	4167	69.4	1.2	0.0
LCLS	Rayonix	10	50000	833.3	13.9	0.6
LCLS	Rayonix	30	16667	277.8	4.6	0.2
SACLA / PAL-XFEL	MPCCD	60	8333	138.9	2.3	0.1
SwissFEL	Jungfrau	100	5000	83.3	1.4	0.1
Eu.XFEL	Jungfrau *	160	3125	52.1	0.9	0.0
Diamond VMXi	Eiger2	500	1000	16.7	0.3	0.0
Eu.XFEL	AGPID	3,250	154	2.6	0.0	0.0
LCLS-II-HE	ePIX *	10,000	50	0.8	0.0	0.0
SHINE	tbd *	17,000	29	0.5	0.0	0.0

indexed images **25,000**

hit ratio = 80%		image rate	time to collect full SFX dataset		
facility	detector	Hz	seconds	mintues	hours
LCLS	CSPAD	120	260	4.3	0.1
LCLS	Rayonix	10	3125	52.1	0.9
LCLS	Rayonix	30	1042	17.4	0.3
SACLA / PAL-XFEL	MPCCD	60	521	8.7	0.1
SwissFEL	Jungfrau	100	313	5.2	0.1
Eu.XFEL	Jungfrau *	160	195	3.3	0.1
Diamond VMXi	Elger2	500	63	1.0	0.0
Eu.XFEL	AGPID	3,250	10	0.2	0.0
LCLS-II-HE	ePIX *	10,000	3	0.1	0.0
SHINE	tbd *	17,000	2	0.0	0.0

Serial MX data collection rates are driven by hit ratio & detector speed

Detector or source speed	Serial MX snap shot
100 Hz (Pilatus)	10 ms
500 Hz (Eiger2)	2 ms
500 Hz + e^- gated	100 µs
10,000 Hz	100 µs
XFEL pulse duration	10 – 50 fs
Eu.XFEL train length	600 µs

Allen M. Orville, Ph.D.
XFEL Hub at Diamond
Diamond Light Source

Pulse Length

SXR needs the shortest bunches

100 as proposed by users but compatible with compact FEL?

J. Phys. B: At. Mol. Opt. Phys. **51** (2018) 032003

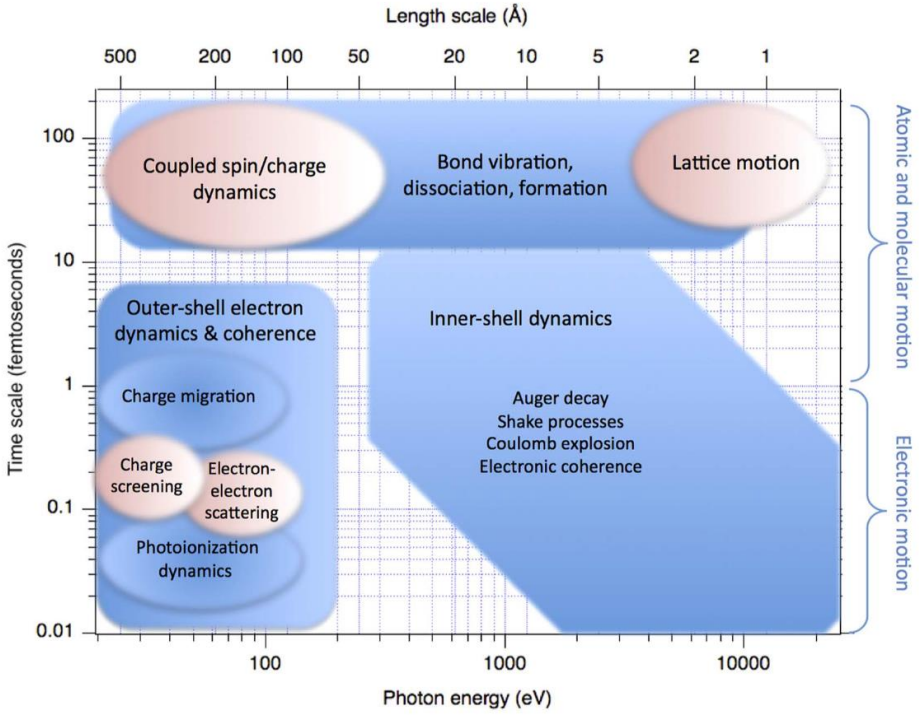

Figure 2. Fundamental atomic, molecular and electronic phenomena probed on ultrafast timescales (blue). Fundamental collective phenomena in the condensed phase probed on ultrafast timescales (pink).

Roadmap of ultrafast x-ray atomic and molecular physics

Linda Young[1,2,22], Kiyoshi Ueda[3], Markus Gühr[4,5], Philip H Bucksbaum[5,6], Marc Simon[7], Shaul Mukamel[8], Nina Rohringer[9,10], Kevin C Prince[11], Claudio Masciovecchio[11], Michael Meyer[12], Artem Rudenko[13], Daniel Rolles[13], Christoph Bostedt[1], Matthias Fuchs[5,14], David A Reis[5], Robin Santra[9,10], Henry Kapteyn[15,16], Margaret Murnane[15,16], Heide Ibrahim[17], François Légaré[17], Marc Vrakking[18], Marcus Isinger[19], David Kroon[19], Mathieu Gisselbrecht[19], Anne L'Huillier[19], Hans Jakob Wörner[20] and Stephen R Leone[21]

Key Parameters To Agree

	Trieste – June 2018	Barcelona – Dec 2018
Max Photon Energy	25 keV	
HXR Repetition Rate	100 Hz	
SXR Repetition Rate	1000 Hz	
Max Pulse Energy	1mJ (@25 keV)	
Minimum pulse duration	100 as	
Bandwidth		