

Self-seeded x-ray free-electron laser with high spectral density and photon energy

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Hard x-ray experiments, such as high-resolution imaging and scattering of complex materials, increasingly demand pulses from x-ray free-electron lasers (XFELs) with high photon energy, high spectral density, and narrow bandwidth. Here, we report the demonstration of hard x-ray self-seeding at 18 keV at the European XFEL. This demonstration narrows the bandwidth to 0.8 eV, compared with 20.5 eV in self-amplified spontaneous emission operation, and increases the average spectral density by a factor of 6, reaching 170 $\mu\text{J}/\text{eV}$ within the same experimental campaign. To advance narrow band operation toward even higher photon energies, we explore the harmonic generation mechanism in self-seeding mode, utilizing the second-harmonic generation self-seeding (SHGSS) scheme, where an initial seed is established at half the target photon energy and the harmonic is coherently amplified downstream. Start-to-end simulations at the 30 keV frontier revealed that while direct self-seeding yielded negligible amplification under typical experimental beam conditions, the SHGSS scheme could deliver an average spectral density of approximately 50 $\mu\text{J}/\text{eV}$ with a 0.25 eV bandwidth using the beamline supplemented with superconducting undulators. With these goals in mind, we experimentally investigated SHGSS at 15 and 18 keV, providing the first proof-of-principle for this scheme. Our results are expected to support cutting-edge experiments in materials science, structural biology, and beyond.

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I. INTRODUCTION

X-ray free-electron lasers (XFELs) have opened frontiers in science by generating ultrabright, coherent, femto-second-scale pulses that are tunable across the hard x-ray regime, enabling direct views into the structure and dynamics of matter at the atomic scale [1–5]. Self-amplified spontaneous emission (SASE) is the dominant lasing mechanism, capable of providing access to photon energies above 10 keV for routine user operations and even 30 keV in test demonstrations at the European XFEL [6,7]. However, its stochastic nature, which originates from the shot noise of the electron beam, leads to multiple temporal

spikes, a broad bandwidth, and poor longitudinal coherence. Although high spectral purity can be obtained in SASE mode, utilizing a monochromator, it comes at the considerable expense of x-ray photon flux.

Many forefront experiments demand x-ray pulses that simultaneously deliver narrow bandwidth, high spectral density, and high photon energy, which cannot be achieved with SASE. A narrow bandwidth is essential for improving the spatial and energy resolutions. In imaging experiments requiring focusing of the beam, the SASE bandwidth causes focal spot broadening when refractive optics is employed and hence degrades the spatial resolution [8]. Photon-hungry applications such as inelastic and resonant x-ray scattering demand high spectral density to compensate for the often small scattering cross section [9]. High photon energies, in turn, are broadly required to penetrate thick or embedded samples [10,11], extend the diffraction-limited spatial resolution (access to high momentum transfers) [12,13], and mitigate radiation damage in crystalline materials [14,15]. A representative example that benefits from all these properties is dark-field x-ray microscopy (DFXM), which typically exploits 25–60 keV synchrotron radiation [16,17] to characterize microstructures in thick, strongly absorbing samples [18] and

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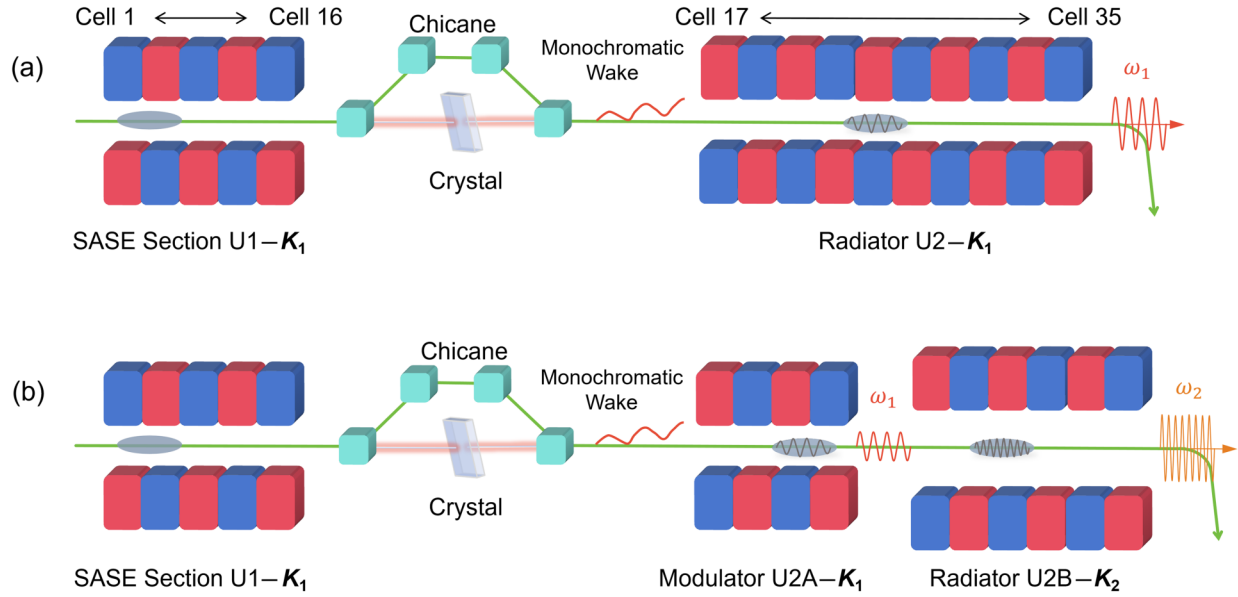


FIG. 1. Schematic layout of the (a) hard x-ray self-seeding system and (b) second-harmonic generation self-seeding system implemented in the SASE2 beamline of the European XFEL. Here, the U1 section comprises 16 cells, while the U2 section consists of 19 cells. Although the SASE2 beamline features two chicane-crystal sets to mitigate heat load, thermal effects are negligible above 8 keV, with no observable shift in the central wavelength [27]. Therefore, only the second chicane-crystal set was utilized in our layout to simplify the setup and preserve the incident pulse energy on the crystal.

demands high flux to resolve weak diffraction signals [19]. The extension of DFXM to XFELs further enables capturing of transient structural states [20]. However, the broad bandwidth of SASE pulses would smear the resolution in elastic strain measurements [19,21], and narrowing the spectrum with crystal-based monochromators at XFELs typically results in a severe reduction of the photon flux, which calls for direct generation of high-spectral-density pulses. Given that such narrow-bandwidth, high-spectral-density XFEL pulses are currently restricted to below 15 keV at most facilities, extending the photon-energy range is thus crucial for the next generation of materials science.

The most widely utilized method to directly produce narrow-bandwidth, high-spectral-density hard x-ray pulses is the hard x-ray self-seeding (HXRSS) technique, a compact scheme based on forward Bragg diffraction (FBD), as proposed in 2011 [22] [Fig. 1(a)]. This approach can yield an average peak spectral density that exceeds that of the SASE mode by several times [23,24], successfully extending spectral purity into the hard x-ray regime. The HXRSS technique has since been verified at multiple facilities and routinely employed in user operations, establishing its reliability and robust performance [23,25–27]. Driven by the need to push beyond the 15 keV photon energy, we explored the effective photon-energy boundary of the standard HXRSS architecture at the European XFEL and extended it up to 18 keV under typical beam conditions, leveraging the high electron-beam energy and the long undulator beamline. However,

pushing direct HXRSS further into the ultrahard x-ray regime is constrained by longer gain lengths, available undulator lengths, and the requirement for extreme electron-beam parameters, such as high peak currents and ultralow emittances.

To bypass these constraints, harmonic generation presents a compelling alternative [28]. Currently, externally seeded harmonic generation schemes, such as high-gain harmonic generation (HGHG) [29–32] and echo-enabled harmonic generation (EEHG) [33,34], are widely utilized. While successful in the soft x-ray regime, extending these externally seeded methods to shorter wavelengths presents significant technical challenges regarding the availability of high-power short-wavelength seed lasers and their limited frequency up-conversion efficiencies [35,36]. These challenges motivate an alternative approach: exploring the harmonic generation mechanism in the hard x-ray self-seeding mode [37,38]. At variance with HGHG and EEHG, we utilize the harmonic bunching related to the nonlinear harmonic generation (NHG) emission in a direct self-seeding setup, leveraging the intrinsic R_{56} of the undulators as the dispersion section, which is particularly suited to hard x-ray. In HXRSS, the self-generated monochromatic seed can easily reach photon energies above 10 keV at the fundamental with megawatt-level power. Therefore, by amplifying this harmonic bunching in a dedicated downstream undulator section, this approach promises to extend spectrally pure, high-spectral-density XFEL pulses into the ultrahard x-ray regime.

As illustrated in Fig. 1(b), this method was initially proposed in Refs. [37,38]. In this paper, we refer to it as the second-harmonic generation self-seeding (SHGSS) scheme. In this approach, the configuration structurally resembles direct self-seeding, but the upstream SASE section is tuned to resonate at the fundamental rather than the target second harmonic. The downstream radiator section is then divided into two parts: the first remains tuned to the fundamental to drive nonlinear harmonic bunching, while the final part is tuned to the target photon energy (the second harmonic) for amplification. Since the gain is mainly contributed by the downstream radiator, this architecture is well suited for the planned installation of superconducting undulators (SCUs) following the current beamline [39,40].

In the following section, we will report a combined experimental and simulation effort to extend the capabilities of hard x-ray self-seeding at the European XFEL. First, we characterized the performance of the standard HXRSS scheme up to 18 keV, experimentally extending its practical photon-energy range under typical beam conditions and establishing it as the highest HXRSS photon energy demonstrated to date. Second, to push beyond the 18 keV boundary, we performed start-to-end simulations at the 30 keV frontier to provide a comparative assessment of HXRSS and SHGSS, highlighting the distinct advantages of the latter in this energy regime. Finally, we experimentally demonstrated the amplification of SHGSS as a proof-of-principle for harmonic up-conversion within self-seeded FEL architectures, offering a viable pathway toward a high-spectral-density, high-photon-energy self-seeded free-electron laser.

II. HARD X-RAY SELF-SEEDING AT HIGH PHOTON ENERGY

The HXRSS system for photon energies above 8 keV is implemented in the SASE2 beamline at the European XFEL, as illustrated in Fig. 1(a). In the upstream undulator section U1, the electron beam generates broadband SASE radiation. U1 comprises 16 undulator cells, each 5 m long with a 40 mm period, separated by 1.08 m intersections that accommodate critical components, including phase shifters, aircoils, and diagnostic devices such as beam position monitors. The x-ray pulse is then sent through an FBD monochromator based on a thin diamond crystal. When oriented to satisfy the selected Bragg condition for the target frequency ν , the crystal acts as a spectral filter that imprints a narrow notch in the SASE spectrum. In the time domain, this corresponds to a delayed, narrow band monochromatic wake, which serves as a coherent seed for the downstream amplification. Simultaneously, the electron bunch passes through a weak magnetic chicane. This chicane provides the transverse offset required for crystal installation and introduces a precisely adjustable electron delay to temporally overlap the electron bunch with the

seed. In addition, the longitudinal dispersion of the chicane effectively suppresses the residual SASE-induced microbunching from U1. Finally, the seeded electron bunch enters the downstream undulator section U2, which comprises 19 cells sharing an identical configuration and segment spacing with U1. In this section, the coherent signal rapidly builds up bunching at the fundamental and undergoes exponential gain, producing a highly coherent hard x-ray pulse with substantially reduced bandwidth.

During daily user operations at the European XFEL, the proportion of user proposals requiring HXRSS has grown to account for up to 50% [24], reflecting a growing demand for narrow bandwidth and high spectral density. However, generating self-seeded pulses whose spectral density exceeds that of monochromated SASE at photon energies above 15 keV presents a considerable challenge.

Taking advantage of the beam energy at 16 GeV, we demonstrated the first HXRSS experiment at 18 keV, marking a significant extension of the self-seeding operational photon-energy range. Figure 2(a) compares the output performance in the SASE and HXRSS modes at 18 keV measured in the same experiment campaign with comparable machine and beam conditions. The spectra were recorded by the high-resolution hard x-ray (HIREX) spectrometer [41,42] (0.52 eV/pixel resolution for this case), located—along with the x-ray gas monitor (XGM) [43,44]—approximately 500 m downstream of the undulator. The total pulse energies were characterized using an XGM, yielding 280 μ J for HXRSS and 700 μ J for SASE, the latter exceeding the average SASE performance at 18 keV. In terms of spectral bandwidth, the HXRSS mode achieved an average full width at half maximum (FWHM) of 0.8 ± 0.25 eV, representing an over 20-fold reduction compared with the 20.5 ± 6.64 eV observed in the SASE mode. The average spectral density over 1000 shots reaches approximately 170 μ J/eV, representing an approximately six-fold increase over the SASE mode.

The self-seeding signal exhibits a spectral pedestal surrounding the central seed, originating from the SASE background, a phenomenon consistently observed across multiple facilities [23,25,27,45]. To quantify this component, the crystal was moved out to suppress seeding amplification; under these conditions, the background contribution was found to account for approximately 50% of the total HXRSS pulse energy. In principle, redistributing the peak current toward the bunch head by optimizing the chirp, curvature, and cubic coefficients of the electron beam could effectively suppress this underlying noise, subsequently enhancing the signal-to-noise ratio and narrowing the spectral bandwidth [46]. However, as the experiment was conducted during machine development shifts, the limited beamtime precluded the full optimization of the pulse performance, leaving this spectral pedestal partially unsuppressed. Nevertheless, the enhancement in spectral density over SASE presents the

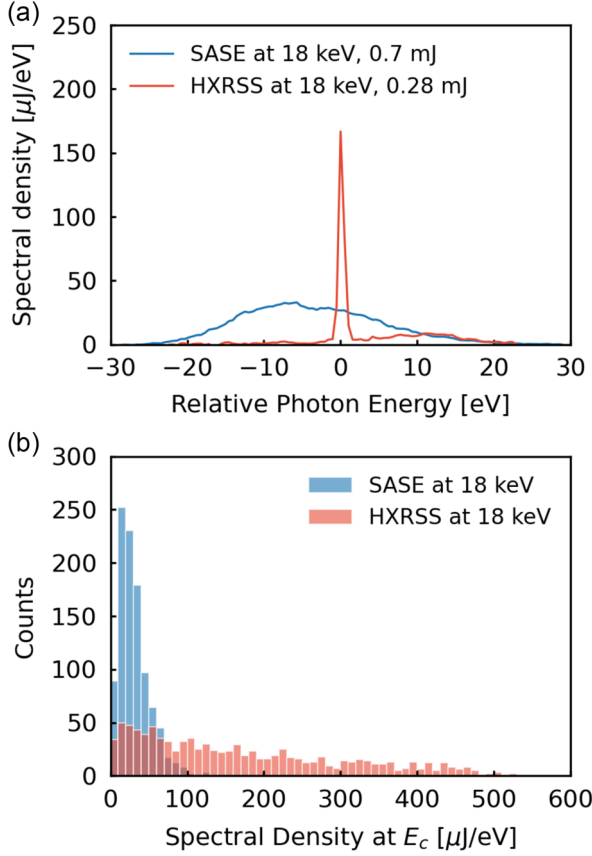


FIG. 2. (a) Experimental average output spectra for the HXRSS and SASE modes, with total pulse energies of 0.28 and 0.7 mJ, respectively. The data consist of 1000 consecutive shots recorded under comparable electron-beam conditions. (b) Statistical distribution of the spectral density with 1000 consecutive shots for the HXRSS and SASE modes at 18 keV. For each mode, the spectral density is evaluated at its central photon energy, which corresponds to the peak of its average spectrum.

robust spectral concentration capability of the self-seeding scheme even under nonideal conditions.

Figure 2(b) presents the statistical analysis of the spectral densities for both HXRSS and SASE modes at 18 keV. In the linear regime, a perfectly seeded photon beam is expected to show the same statistics as a single-mode SASE pulse: a negative exponential distribution with 100% fluctuations ($M \approx 1$, $\sigma^2 \approx 1/M$) [47]. At variance with this ideal case, here we observe that the HXRSS distribution is characterized by a long tail with 78% shot-to-shot fluctuations. The HXRSS signal remains in the linear gain regime, as the available amplification length was limited by nonideal undulator alignment and orbit conditions: all 16 cells in U1 were utilized to deliver approximately 25 μJ to the crystal, and only 13 cells in U2 contributed to the seeded amplification. In contrast, the SASE distribution follows a Gaussian-like profile with reduced fluctuations of 65%.

For harder x-ray regimes, the increased gain length at higher photon energies demands a longer upstream SASE section to generate sufficient pulse energy and seed power. Within the fixed undulator budget, this inevitably reduces the downstream radiator length and degrades the spectral density, a fundamental trade-off that becomes increasingly severe as the target photon energy rises. Consequently, while we demonstrated direct self-seeding at 18 keV with high spectral density, extending it to even higher photon energies faces hardware limitations.

III. TOWARD SELF-SEEDING AT 30 KEV

Motivated by the demonstration of SASE operation at 30 keV with meticulously tuned, ultralow emittance electron beams at the European XFEL [6], we aim to explore whether seeded operation at this photon energy can be achieved using typical electron-beam parameters. The direct self-seeding simulation at 30 keV indicates insufficient gain, as discussed in Appendix A. To this end, we employ the SHGSS scheme, which relaxes the upstream undulator requirements and shifts the primary amplification to the downstream section. In this section, we present start-to-end simulation results of the SHGSS scheme at 30 keV.

The input electron-beam phase-space distribution was generated with the multiphysics software package OCELOT [48]. The electron bunch was accelerated and longitudinally compressed to reach a kiloampere-level peak current, while collective effects during acceleration and compression, such as coherent synchrotron radiation (CSR) and longitudinal space charge, were taken into account. During the linac rf and bunch compressor setting optimization, an iterative approach was utilized to converge on a typical, realistic machine condition [46]. The resulting 6D macroparticle distribution was then transported through the switchyard and matched to the entrance of the SASE2 undulator. Because of the CSR effect induced by the switchyard, the input beam exhibits a considerable transverse offset [49]. This realistic distribution serves as the foundation for all subsequent simulations. Starting from the undulator entrance, the lasing process was simulated using the OCELOT framework coupled to Genesis 1.3 [50] for time-dependent FEL calculations. The beam longitudinal profiles are shown in Appendix A. The beam parameters and the hardware setup for both configurations at 30 keV are shown in Table I. As listed in the table, the extension represents the SCU afterburner at the end of SASE2, which provides an additional 24 m of magnetic length.

As illustrated in Fig. 1(b), we implement the SHGSS scheme, which reconfigures the existing HXRSS infrastructure for second-harmonic operation. To reach demanding photon energies, the upstream SASE radiator is tuned to the fundamental resonance at half the target frequency ($\nu/2$), which facilitates the generation of an

TABLE I. Electron-beam parameters, system setup, intermediate metrics, and radiation performance for the SHGSS configuration at 30 keV. U1 and U2A are tuned to 15 keV, while all other sections resonate at 30 keV. $I_{\max}$ is the spectral density at the central photon energy, and bandwidth refers to the FWHM bandwidth.

Parameters	Values	Units
<i>Electron beam parameters</i>		
Beam energy, E_{beam}	16.1	GeV
Beam charge	250	pC
Slice energy spread, σ_E	2	MeV
Peak current, I_{pk}	4.3	kA
Emittance, $\varepsilon_{n,x/y}$	0.35/0.4	mm mrad
<i>Undulator and crystal setup</i>		
U1	1–11	/
Crystal reflection	C444	/
U2A	17–25	/
U2B	26–35	/
Extension undulators	36–40	/
<i>Intermediate metrics</i>		
Pulse energy after U1	17	μJ
Average wake peak power, P_{wake}	0.1	MW
Bunching factor at 30 keV after U2A	4	%
<i>Radiation performance after the U2B–extension undulators</i>		
Average $I_{\max}$	48.1	$\mu\text{J}/\text{eV}$
$I_{\max}$ jitter	99.7	%
Average bandwidth	0.25	eV
Gain length, L_g	10.59	m

input seed. For instance, in our subsequent simulation targeting 30 keV, the fundamental seed is generated at 15 keV. The FBD monochromator and magnetic chicane then process this fundamental seed pulse in the same manner as in the direct self-seeding configuration.

The key difference arises in the downstream amplification section U2. The initial undulator cells, U2A, are tuned to resonate at $\nu/2$. In this section, the interaction between the seeded signal and the electron beam drives the formation of microbunching not only at the fundamental but also at higher-order harmonics, resulting in NHG emission. Once the harmonic bunching is sufficiently established, the resonance of the subsequent cells, U2B, is shifted to the target frequency ν . The second-harmonic density modulation then acts as the input source for U2B. For a short U2B comprising only a few cells, the system behaves merely as a radiator for a coherent harmonic generation (CHG) setup, while an extended U2B enables an effective FEL process to be established, exponentially amplifying the initial density modulation.

Regarding the SHGSS configuration, 11 out of 16 cells were used in the upstream section U1 to generate an incident SASE pulse with an energy of 17 μJ . This number

of SASE cells was carefully optimized: fewer cells would result in insufficient wake power to induce adequate density modulation in U2A, while more cells would lead to excessive SASE radiation and increase the slice energy spread, thereby degrading the beam quality required for efficient second-harmonic emission in U2B. The crystal plane was set to the diamond C444 reflection, which is discussed in detail in Appendix B. After the crystal, the transmitted radiation wake exhibits characteristic temporal oscillations. To maximize the available monochromatic wake power and minimize the impact of SASE fluctuations, the first wake peak was utilized, with an average peak power of 0.1 MW.

In the downstream modulator section U2A, nine undulator cells were used to establish harmonic microbunching, resulting in a second-harmonic bunching factor of approximately 4% at the entrance of U2B, which starts at cell 26. Similar to the U1 section, this choice represents a trade-off between generating sufficient harmonic bunching and preserving the beam quality for subsequent amplification. The intermediate metrics are listed in Table I.

Figure 3(a) illustrates the evolution of the average spectral density over 100 pulses at the central photon energy along the undulator line of SHGSS. At the exit of the current SASE2 beamline (cell 35), the SHGSS mode has not yet reached saturation and continues to grow, which would be advantageous in case a downstream extension of the undulator length is planned. The average spectral density reaches approximately 50 $\mu\text{J}/\text{eV}$ after extension cells. The average FWHM is about 0.25 eV, and the fluctuation of spectral density is 99.7%, consistent with single-mode statistics in the linear gain regime.

Figures 3(b) and 3(c) display representative single-shot results for the SHGSS mode at the end of undulator extension, showing the slice energy spread and second-harmonic bunching factor, alongside the single-shot output spectra and their average profiles. According to the simulated lasing window and bandwidth, the time-bandwidth product is 1.37 times the transform limit of a Gaussian beam, indicating a high degree of longitudinal coherence. However, the output spectrum still exhibits some minor sidebands. These arise because, in the time domain, while the seed signal is predominantly a monochromatic wake, its leading edge still contains residual broadband SASE components, and the input electron beam possesses an energy chirp. These residuals induce density modulation at off-resonant frequencies. This effect can be mitigated by tailoring the electron bunch current profile to shift the peak-current region further away from the SASE background [46]. Furthermore, in these simulations, a beam with realistic conditions was employed, which can be optimized in future operations to enhance the output intensity.

The main conclusion to be drawn from our simulation is that combining self-seeding with harmonic generation

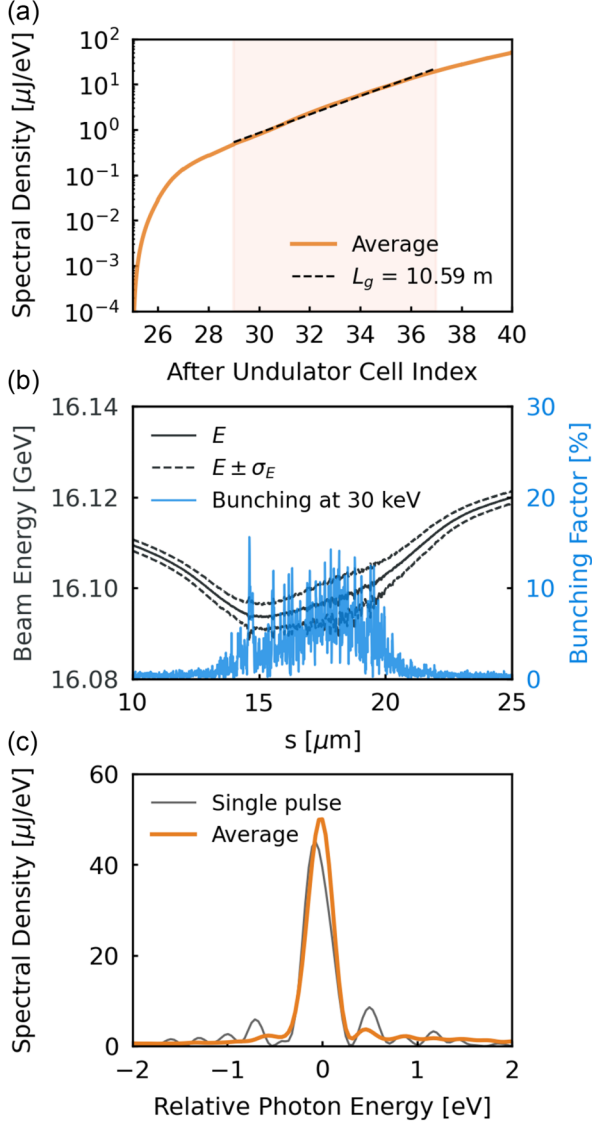


FIG. 3. Simulated results for the SHGSS scheme at 30 keV. (a) The average spectral density at the central photon energy along the U2B undulator beamline, averaged over 100 pulses. The U2B radiator section begins at cell 26, with an exponential-gain regime spanning from cell 29 to 37. (b) Slice energy spread and bunching factor profiles along the electron bunch for a representative simulated shot after cell 40. (c) Single-shot for the same representative shot and average spectra after cell 40.

represents a scalable approach to produce high-spectral-density pulses at photon energies well beyond the current HXRSS range.

IV. SECOND-HARMONIC GENERATION SELF-SEEDING DEMONSTRATION

Given the above results, we experimentally demonstrated the amplification process of this scheme as a proof-of-principle. With fundamental energies of 7.5 and 9 keV,

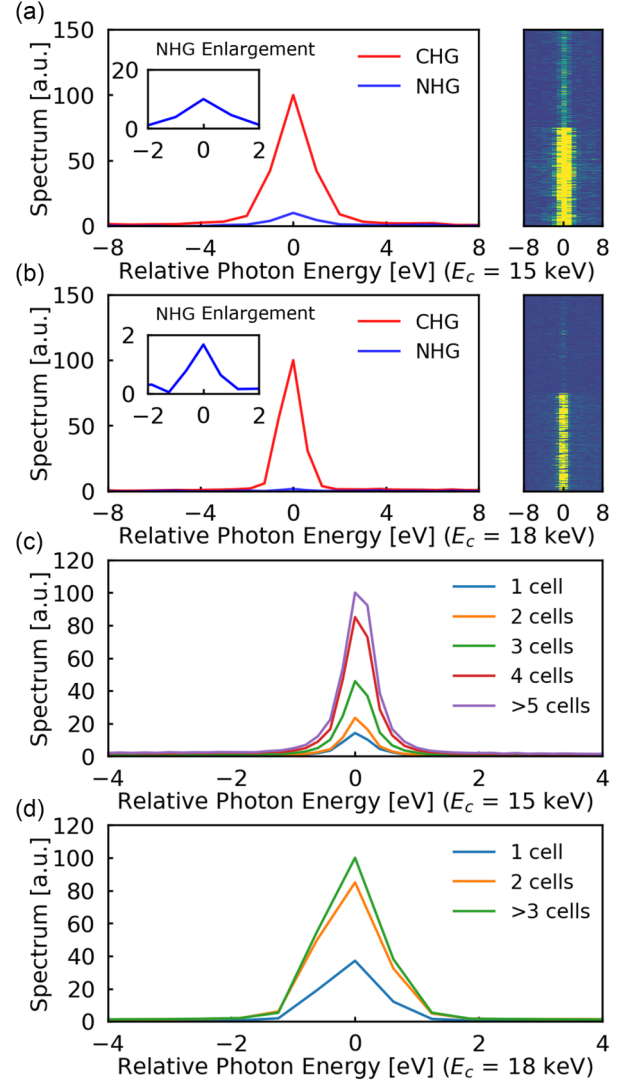


FIG. 4. Experimental results for the SHGSS scheme at 15 and 18 keV. (a and b) Average spectra and single-shot spectral waterfalls over 600 shots measured at (a) 15 and (b) 18 keV during SHGSS operation, showing the transition before and after activation of the first U2B undulator cell. Each average spectrum shows the CHG component (lower 300 shots, after activation) and the NHG component (upper 300 shots, before activation), with an inset zooming in on the NHG spectrum. Time runs from top to bottom. (c and d) Measured second-harmonic spectra, averaged over 1000 consecutive shots, for varying numbers of active U2B cells at (c) 15 and (d) 18 keV.

Figs. 4(a) and 4(b) show the experimental observation of self-seeded second-harmonic generation at 15 and 18 keV, respectively. The left panels of these figures compare the averaged spectra of the NHG and CHG signals, while the right panels show the corresponding single-shot spectral waterfalls recorded by the HIREX spectrometer as the first U2B undulator is switched to the second harmonic.

Experimentally, when U2B is inactive, with the undulator cells at maximum gaps, the weak signal measured at the second harmonic originates from nonlinear harmonic generation in U2A and is therefore denoted NHG. After U2B is tuned to the second-harmonic resonance, this preexisting harmonic microbunching seeds coherent amplification in U2B, producing the CHG signal with a pronounced enhancement of the spectral intensity. This clear signal growth, evident in both the averaged spectra and the single-shot waterfall plots, directly confirms that the harmonic microbunching drives the subsequent FEL amplification. The consistent behavior observed at both photon energies exhibits the feasibility of harmonic up-conversion under hard x-ray self-seeded conditions, laying the groundwork for extension to higher photon energies.

Following the observation of the initial harmonic signal amplification, the optimization was conducted as detailed in Appendix C. Figures 4(c) and 4(d) display the HIREX spectra at 15 and 18 keV after optimization for varying numbers of active U2B cells, with each spectrum averaged over 1000 consecutive shots. Note that the starting position of the radiator U2B section varies depending on the target photon energy: it begins at cell 24 for 15 keV (using seven U2A cells at 7.5 keV for bunching), but at cell 26 for 18 keV (using nine U2A cells at 9 keV). This is consistent with the expectation that higher photon energies possess longer gain lengths, demanding more U2A cells for microbunching growth and thus shifting the U2B onset to a later cell. From the figure, the amplification rate degrades after five cells at 15 keV and three cells at 18 keV, which is attributed to the suboptimal beam alignment and orbit deviations introduced during the photon-energy transition, leaving room for further improvement in future experiments. As demonstrated by the simulations in Appendix C, with an idealized electron-beam orbit, the 15 keV SHGSS signal rapidly enters the exponential-gain regime in U2B and reaches saturation after 10 radiator cells, reducing the spectral-density jitter from 98% to 51% and thereby potentially improving data-acquisition efficiency.

To evaluate the performance under the current trajectory limitations, a quantitative assessment of the generated harmonic pulse energy was necessary. In the second-harmonic configuration, the radiation output comprises a mixture of fundamental and second-harmonic components. Since the XGM measures the total photon flux without spectral discrimination, the harmonic pulse energy cannot be directly extracted from its readings.

We employed a cross-calibration method based on the HIREX spectra to determine the pulse energy of the second-harmonic component (e.g., at 15 keV), as described in Appendix D. Using this procedure, the calibrated pulse energy at 15 keV was estimated to be about 14 μ J with five U2B cells, as shown in Fig. 5. The

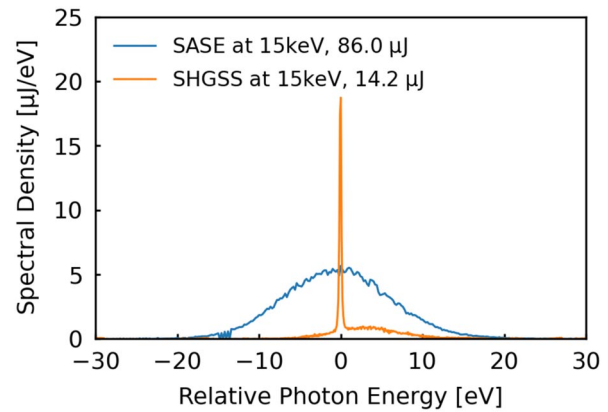


FIG. 5. Experimental output spectral signals of the SASE and SHGSS schemes at 15 keV. The SHGSS pulse energy is calibrated to 14.2 μ J with five U2B cells closed. Note that the SASE configuration was used solely as a calibration reference and was not tuned to saturation.

peak spectral density reached approximately 18 μ J/eV, with shot-to-shot fluctuations of 57%, evaluated at a HIREX resolution of 0.62 eV/pixel. As detailed in Appendix C, simulations of SHGSS at 15 keV predict a spectral density of 15 μ J/eV after four U2B cells, in reasonable agreement with the experimentally observed value after five cells, and project an average spectral density exceeding 500 μ J/eV, when all cells contribute. Although in this experimental demonstration the output has not yet been fully optimized, this work represents, to our knowledge, the first amplification of harmonic generation under hard x-ray self-seeded operation.

V. CONCLUSION AND DISCUSSION

In summary, we have extended the operational envelope of hard x-ray self-seeding at the European XFEL to a record photon energy of 18 keV, yielding an average peak spectral density of 170 μ J/eV and a bandwidth of 0.8 eV. Both experimental observations and start-to-end numerical studies indicate that direct self-seeding is approaching its practical limit at elevated photon energies, primarily constrained by the available upstream undulator length required to generate sufficient monochromatic wake power. To overcome this boundary, we proposed and implemented the SHGSS scheme. By initiating the SASE and subsequent seeding processes at a lower fundamental frequency, SHGSS effectively decouples the initial seed generation from the final high-energy amplification. We presented the potential of this approach through numerical studies at 30 keV and demonstrated its experimental feasibility at 15 and 18 keV. As the European XFEL continues to evolve with extended undulator sections and advanced magnetic structures, the efficiency and spectral brightness of the SHGSS configuration will be further

enhanced. This demonstration paves the way for future high-energy operations at other facilities, such as the Shanghai hard x-ray facility, which will incorporate a self-seeding beamline equipped with 42 undulator cells [51].

Looking ahead, fully unlocking the SHGSS scheme requires addressing the following challenges. The coherent harmonic amplification was found to be sensitive to orbit deviations induced by undulator K -value transitions. Developing automated, localized photon-beam-based alignment procedures [52], coupled with enhanced downstream orbit feedback, will enable full exploitation of the available undulators. By addressing these trajectory sensitivities, alongside the planned SCU integration and the ongoing efforts to minimize beam emittance [6], the SHGSS configuration will be capable of delivering high-purity pulses without severe intensity losses and optical setup associated with conventional postundulator monochromators.

Ultimately, integrating self-seeding with harmonic generation offers a promising and practical route to meet the growing scientific requirements for high-photon-energy, high-spectral-density hard x-ray beams. This capability is well suited to support demanding applications in high-resolution spectroscopy and structural dynamics at extreme photon energies.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

APPENDIX A: START-TO-END NUMERICAL SIMULATION OF HXRSS AT 30 KEV

Figure 6 shows the electron-beam properties at the undulator entrance used for both HXRSS and SHGSS

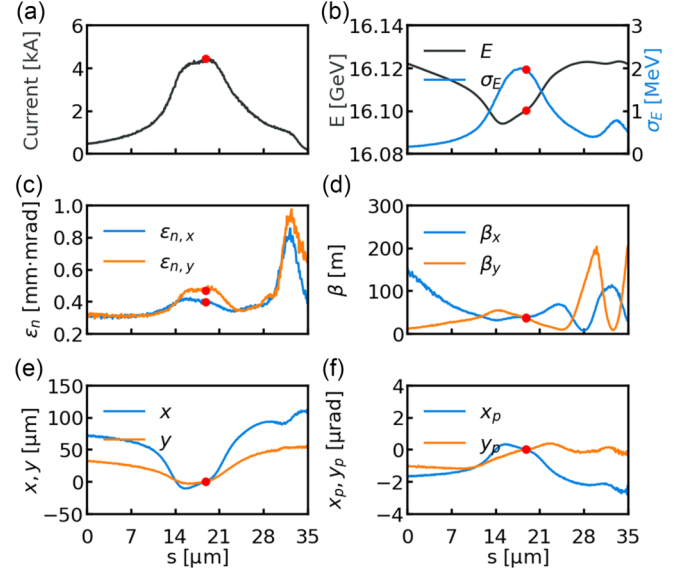


FIG. 6. Electron-beam properties at the entrance of the U1 section used in simulations for the HXRSS and SHGSS configurations. The red dot marks the peak-current slice used for transverse-optics matching. The beam head is to the right. (a) Longitudinal current profile along the bunch. (b) Slice beam energy and slice energy spread. (c) Normalized transverse emittance in the horizontal and vertical planes. (d) Beta functions in the horizontal and vertical planes. (e) Transverse centroid offsets. (f) Transverse angular divergence.

schemes. For the HXRSS scheme, the existing 16 cells were insufficient to generate adequate incident pulse energy at 30 keV. Consequently, we extended the U1 section by four virtual cells in the simulation to reach an incident pulse energy of 30 μ J, achieving a seed power of 0.6 MW at the target photon energy using the diamond C444 reflection (see Appendix B). We utilized all the U2 and extension undulators for the amplification of seeding at 30 keV.

Figure 7 illustrates the output performance of the HXRSS scheme after the extension section. It is evident that the seed power of 0.6 MW is still insufficient for direct amplification at 30 keV under the given beam parameters, even when utilizing 20 cells for the incident SASE generation. Although the bunching factor at 30 keV has reached 15% across all undulator cells and the output pulse energy from downstream is approximately 30 μ J, the spectrum is highly chaotic and dominated by numerous spectral spikes, indicating that the amplification of the seed is small. Consequently, unless significantly improved beam parameters are achieved, extending the standard HXRSS scheme to higher photon energies is challenging.

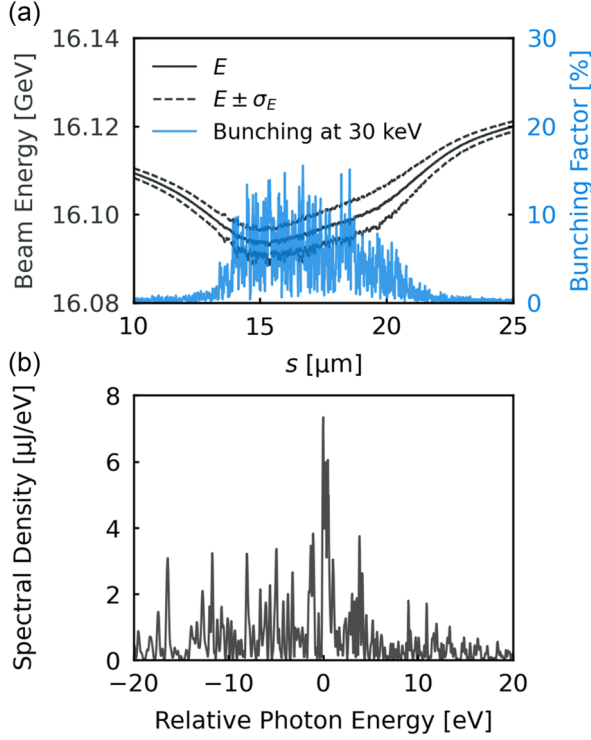


FIG. 7. Simulated results for the HXRSS scheme at 30 keV. (a) Slice energy spread and bunching factor profiles along the electron bunch for an optimized shot after cell 40. (b) The spectrum of the optimized shot after cell 40. Note that the HXRSS simulation includes four additional virtual cells in the upstream SASE section to provide enough seed power, bringing the total to 44 cells.

APPENDIX B: CRYSTAL REFLECTION PLANES OF HXRSS AND SHGSS AT 30 KEV

For HXRSS at 30 keV, we used the diamond C444 reflection, which corresponds to a pitch angle of 26.6° at 30 keV. Figure 8(a) shows the longitudinal power profile of the monochromatic wake at 30 keV for the direct self-seeding scheme. Here, we pick the first wake to overlap with the peak-current position, and the corresponding seed power is about 0.6 MW.

Figure 8(b) illustrates the temporal wake power profiles generated by various crystal reflections driven by the same SASE pulse at 15 keV. Theoretically, the duration of the monochromatic wake is inversely proportional to the crystal's Darwin width. Our simulations reveal that the peak power of the first wake oscillation follows this expected decreasing trend for higher-order planes. However, most evaluated reflections, with the exception of the C337 plane, sustain a primary peak power exceeding 0.3 MW. Consequently, the C444 configuration was selected, which exhibits the flattest wake and provides the highest average power across the beam bunch length.

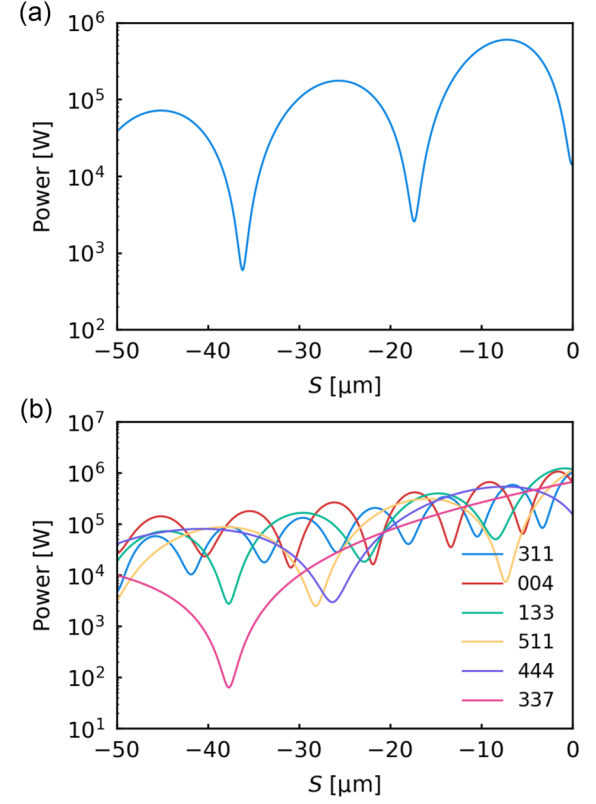


FIG. 8. Simulated longitudinal power profiles of the monochromatic wakes. (a) The 30 keV wake generated via the diamond C444 reflection for the standard HXRSS scheme. (b) The 15 keV fundamental wakes generated across various crystal reflection planes for the SHGSS scheme targeting 30 keV, all driven by the same initial SASE pulse. Here, the zero point on the x axis denotes the onset of the monochromatic wake.

APPENDIX C: EXPERIMENTAL OPTIMIZATION PROCEDURE FOR THE SHGSS SCHEME AND SIMULATION PERFORMANCE DEMONSTRATED AT 15 KEV

Following the initial observation of the harmonic signal, we systematically optimized it in the experiment. First, we adjusted the starting point of the U2B radiator to achieve the highest spectral peak signal, striking a balance between inducing sufficient harmonic bunching and preserving the electron-beam quality for the subsequent amplification. Then, we conducted the cell-by-cell scan of the interundulator phase shifters. Furthermore, we applied the Generic Optimizer [53] to optimize the aircoil settings in the U2 section, using the HIREX peak signal as the optimization objective. Concurrently, the electron beam launch trajectory at the U2B entrance was carefully fine-tuned.

Simulations were also conducted for the SHGSS mode at 15 keV to compare with experimental results and validate the realism of the simulated electron-beam profile. The simulation used the same electron-beam

TABLE II. Simulated and experimental electron-beam parameters and system setup for the SHGSS configurations at 15 keV. Here, U1 and U2A resonate at the fundamental harmonic, while U2B resonates at the second harmonic.

Parameter	Simulation	Experiment	Units
<i>Electron beam parameters</i>			
Beam energy, E_{beam}	14.0		GeV
Beam charge	250		pC
Peak current, I_{pk}	4.3		kA
Emittance, $\epsilon_{n,x/y}$	0.35/0.4		mm mrad
<i>Undulator and crystal setup</i>			
U1	1–8	1–13	/
Crystal reflection		C004	/
U2A	17–22	17–23	/
U2B	23–35	24–35	/

distribution and parameters, as described in Sec. III, except that the beam energy was adjusted to 14.0 GeV, as listed in Table II.

The diamond crystal reflection is C004, corresponding to a pitch angle of 114° at the 7.5 keV fundamental energy, which is identical to the experimental setting. The chicane delay was scanned to optimize the temporal overlap between the first monochromatic wake and the peak-current region of the electron bunch. This configuration yields an average peak wake power of approximately 0.5 MW, sufficient to initiate microbunching.

In the downstream section, the modulator U2A employs six cells, producing a second-harmonic bunching factor of approximately 5% at the entrance of U2B. Since U2 consists of 19 cells in total, 13 cells remain available in U2B for harmonic gain.

Figure 9 illustrates the evolution of the average spectral density at the central photon energy along the undulator cells. In this case, the U2A section ends at cell 22, while the U2B radiator starts at cell 23. By cell 24, the pulse enters the exponential gain regime with a gain length of approximately 5.1 m for the central spectral density, ultimately reaching saturation at cell 32. The insets show the averaged and single-shot spectra at cell 26 and cell 32, exhibiting an FWHM bandwidth of approximately 0.3 eV. Since the simulation assumes an idealized orbit, the experimental amplification is expected to require a slightly larger number of cells to reach a comparable gain level. Consistently, the simulated spectral density after four U2B cells is roughly 15 $\mu\text{J}/\text{eV}$, in good agreement with the experimental value observed after five cells. At saturation, the simulated average spectral density reaches over 500 $\mu\text{J}/\text{eV}$, and the spectral-density jitter drops from 98% to 51%. This reduction is associated with a narrower pulse-to-pulse spectral-density distribution and a larger mean-to-maximum spectral-density ratio. These features are particularly valuable for dose-sensitive experiments,

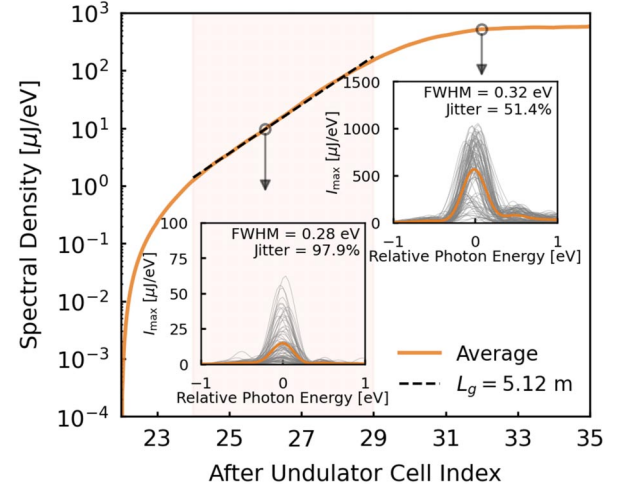


FIG. 9. Simulated results for the SHGSS scheme at 15 keV. The average spectral density at the central photon energy is plotted along the U2B undulator beamline, averaged over 100 pulses. The U2B radiator section begins at cell 23, and the gain length of the central spectral density is approximately 5.1 m. The insets show the single-shot and averaged spectra extracted after undulator cells 26 and 32, respectively.

because they reduce the influence of rare high-intensity pulses on the attenuation required to avoid irreversible sample damage, thereby allowing a larger fraction of the pulses to be used for data acquisition. Together, these results highlight the importance of fully exploiting the available radiator length to reach saturation and illustrate the potential of the SHGSS scheme with a well-optimized electron-beam orbit.

APPENDIX D: PULSE ENERGY CALIBRATION OF SHGSS SCHEME AT 15 KEV

This section describes the pulse-energy calibration procedure for harmonic generation self-seeding, as the upstream XGM (located 500 m downstream of the undulator) measures a mixture of the fundamental and harmonic signals and cannot resolve them directly.

First, HIREX was configured for 15 keV operation in the SASE mode. Under two well-defined attenuation settings (molybdenum filters installed upstream of HIREX), the corresponding upstream XGM pulse-energy readouts and a series of single-shot HIREX spectra at 15 keV were recorded simultaneously as reference data.

Subsequently, the second-harmonic mode was optimized at 15 keV and HIREX spectra were acquired under the identical attenuation settings. For each shot, the central photon energy was defined as the energy at the maximum of the averaged HIREX spectrum. The spectral intensity was then integrated within a symmetric energy window centered at this value, using ± 30 eV for the SASE reference data and ± 20 eV for the SHGSS data to cover both the harmonic peak and the residual SASE spectral

pedestal. The averaged integrated signal over 1000 shots was further used to transfer the absolute energy scale from the SASE reference to the second-harmonic data via the ratio of integrated HIREX signals. The second-harmonic pulse energy was calculated as follows:

$$E_{\text{SHGSS}} = E_{\text{SASE}} \times \frac{\mathcal{I}_{\text{SHGSS}}}{\mathcal{I}_{\text{SASE}}},$$

where E_{SASE} is the upstream XGM pulse-energy readout in SASE mode and $\mathcal{I}_{\text{SASE}}$ and $\mathcal{I}_{\text{SHGSS}}$ are the averaged integrated HIREX signals in SASE and SHGSS modes, respectively. The calibrated harmonic pulse energy is 14.2 μJ , which serves as the basis for calculating the spectral density shown in Fig. 5.

Finally, the calibration was cross-checked by varying the beam transmission through the tunnel to the downstream XGM. The tunnel attenuators were adjusted step-wise, and for each setting, the transmission coefficients at 7.5 and 15 keV were recorded together with the pulse-energy readout from the downstream XGM, which is located near the experimental hutch. The downstream XGM was operated with the Huge Aperture Multiplier detector, which provides sufficient single-shot signal-to-noise ratio at high photon energies. When the transmission coefficient at 7.5 keV is sufficiently low (i.e., below 10^{-3}), the downstream XGM readout is a direct measurement of the 15 keV pulse energy alone. Measurements were performed at three attenuation settings satisfying this condition. From these measurements, the 15 keV pulse energy was derived as $15.2 \pm 1.3 \mu\text{J}$, which is in good agreement with the value obtained from the spectral calibration.

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