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SLAC MeV ULTRAFAST ELECTRON DIFFRACTION FACILITY UPGRADE PLANS*

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Abstract

Mega-electronvolt ultrafast electron diffraction (MeV-UED) is a complementary tool to X-ray based instruments that has enabled ground-breaking studies in condensed matter physics and chemical science. The SLAC MeV-UED facility uses a state-of-the-art 1.6-cell RF photoinjector to deliver 3 to 4 MeV electrons for a variety of pump-probe studies in solids, liquids, and gases, with over 6600 delivered hours and >87 publications since 2021. To broaden the scientific opportunities, facility expansion and enhanced instrument performance of MeV UED have been heavily requested. We discuss near and long-term plans for upgrade and expansion of MeV-UED, with improvements in user delivery, system performance, data acquisition, and temporal and momentum-space resolution.

INTRODUCTION

The MeV-UED instrument at SLAC began operating in 2014 and has since been developed into a powerful tool for understanding molecular structural dynamics and the coupling of electronic and nuclear motions in a variety of material and chemical systems. In 2019, MeV-UED became a user facility as an instrument of LCLS, and since then MeV-UED has dramatically exceeded performance expectations, both in capability and scientific production. Driven by a broad array of collaborating teams at SLAC and around the world, the MeV-UED instrument has enabled over 71 publications since 2019, the majority in high-impact journals including four publications in *Science* and two in *Nature*, together with four PhDs. With strong DOE support, SLAC's MeV-UED facility has brought about a new paradigm in ultrafast electron diffraction and made significant contributions to the DOE Basic Energy Science mission to understand and ultimately control matter and energy at the electronic, atomic, and molecular levels. However, continuing performance enhancements to the MeV-UED instrument are needed to remain at the scientific and technological forefront [1]. We are developing a phased R&D approach that includes designing a higher brightness electron source for MeV-UED to allow for substantial near-term improvements in time and momentum-space resolution, and setting the stage for future expansion of the facility to include a second user beam line.

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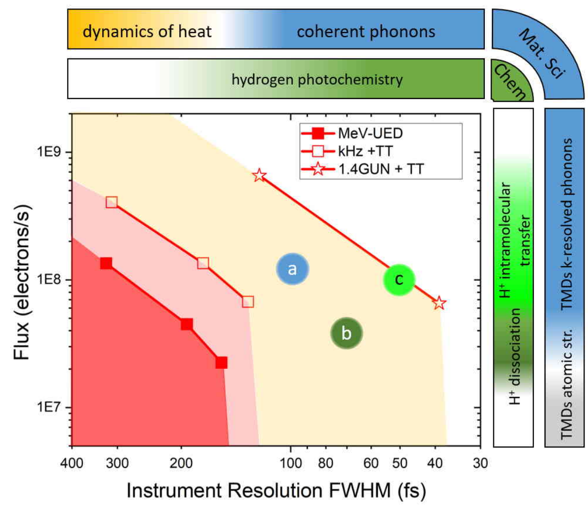

Figure 1: Current and future operational envelopes for the MeV-UED instrument. Solid squares & red region show the current MeV-UED flux/time operation boundary. Open squares & light-red region show the projected performance of MeV-UED with 1 kHz operation and a 1st generation time tool (TT). Open stars & yellow region show the performance of the proposed 1.4 cell gun together with a time tool and pump laser compression. Three specific example science cases are identified: (a) k-resolved transient phonon measurement of mono-layer WSe_2, (b) photodissociation of ammonia, and (c) intramolecular proton transfer in 2-nitrophenol.

SCIENCE DRIVERS AND ENABLERS

The SLAC MeV-UED facility has cultivated a diverse program addressing cutting-edge science across the Basic Energy Sciences portfolio which has capitalized on UED's intrinsic advantages of high cross section, low damage/energy deposition, and its access to both nuclear and electronic atomic distributions. The MeV-UED user workshop held at SLAC in September 2022 and the MeV-UED instrument workshop held in March 2023 identified three key improvements to keep the SLAC MeV-UED at the scientific forefront:

- Improve the instrument sensitivity via increased electron flux and single electron detection.
- Reduce the instrument time resolution below 150 fs towards a goal of 50 fs.
- Lower the transverse beam emittance to enable micro-focused beams and to reach a momentum resolution of $\Delta q = 0.01\ \text{Å}^{-1}$.

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A significant opportunity exists for MeV-UED beyond the current horizon of instrument capability in quantum materials, future microelectronics and photo-chemical research. Figure 1 shows the flux–time operation boundary of current MeV-UED instrument together with the proposed improvements. The improvements in sensitivity and time resolution would enable hydrogen dynamics to be tracked in photochemistry, both for dissociative reactions and for intra-molecular hydrogen transfer. Similarly in microelectronics, an MeV-UED with enhanced time resolution and sensitivity would allow new understanding of the ultrafast processes governing bi-layer conductivity where processes such as charge transfer are enabled by phonon emission in sub-hundred-femtosecond timescales [2]. Further, improvement in transverse emittance would allow access to longer-range electron correlations in quantum materials, going beyond the approximately 3 nm range currently available, to open new areas such as UED application to dynamic Moiré lattice physics in 2D materials. Improved transverse emittance would also enable micro-probe UED allowing the isolation of micron-sized homogeneous regions within complex heterogeneous real-world materials. These improvements would allow MeV-UED to remain at the forefront of cutting-edge science.

NEAR-TERM R&D PRIORITIES FOR MeV-UED

In this section we outline our plans to address the required improvements in sensitivity, time resolution and transverse emittance of the MeV-UED facility. Improvements in the instrument sensitivity are underway [3]. The MeV-UED pump-probe pulse rate has been recently increased from 360 Hz to 1080 Hz enabling a three-fold improvement in electron flux. In addition, a first generation SLAC ePix detector has been commissioned at the instrument capable of single-electron counting at 360 Hz. An extended version of this detector capable of 1080 Hz operation has been recently constructed and is planned for commissioning in FY26. Improvements in time resolution and transverse emittance require an increase in 5D brightness of the electron source by over an order of magnitude as well as a comparable reduction in electron time-of-arrival uncertainty to below 20 fs. To these ends, we are developing a 2-pronged approach for near-term capability enhancement of the facility over the next 2-3 years.

New High-Brightness Electron Source

A project to design a new gun for UED has been recently approved in FY26 under SLAC Laboratory Directed Research and Development (LDRD) funding. The existing MeV-UED electron gun is based on the LCLS design which uses a 1.6-cell geometry and a polycrystalline coppper cathode optimized for >100 pC bunch charge and ps-level bunch durations at LCLS. Extensive simulation studies carried out at MeV-UED using a multi-objective genetic algorithm (MOGA), see Fig. 2, show that a 1.4-cell electron gun design tailored to a UED-specific parameter space (ultra-low charge, high rep rate) could provide as much as a factor of 4 reduction in emittance and a bunch duration below 10 fs at the sample plane, corresponding to more than a factor of 50 improvement in 5D beam brightness. These improvements owe to a modified phase profile in the gun which allows the electrons to see a higher accelerating field upon emission, thereby locking in space-charge earlier and reducing space-charge emittance growth. The resulting higher chirp imparted to the longitudinal phase space additionally provides for bunch compression in the gun without need for additional RF-based or magnetic compressors that can exacerbate jitter and emittance degradation. The proposed approach is similar to well-studied prior art [4], uses well established RF technology, and is compatible with the existing beam line layout and RF system, allowing for a direct swap-out replacement of the existing gun. Combining this approach with a vacuum load-lock system would allow for non-disruptive cathode replacement and additionally allow for exploring various alternative low mean thermal energy (MTE) cathode materials for further reduction in beam emittance.

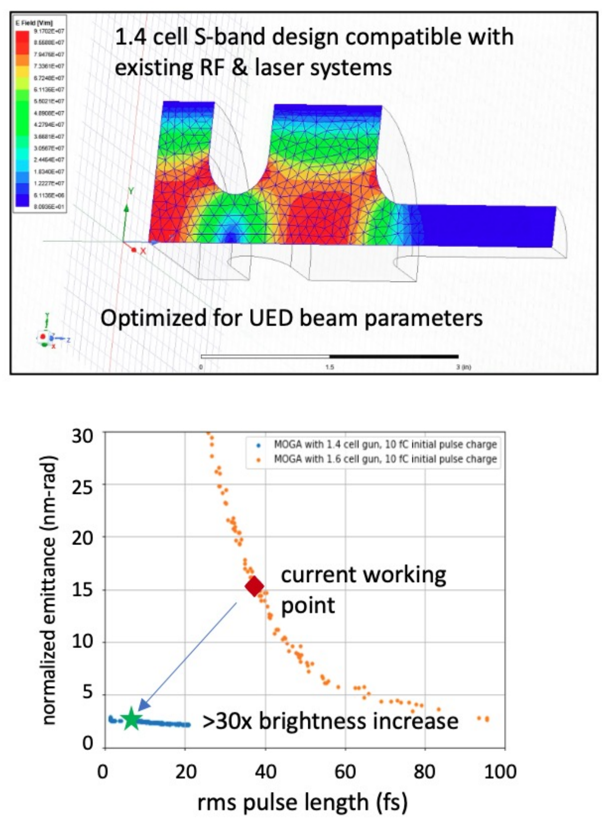

Figure 2: Simulational model of 1.4 cell gun (top panel) and corresponding electron beam emittance vs. pulse length (bottom panel) obtained using multi-objective Bayesian optimization (MOBO) predicts significant 5D brightness improvement is achievable (green star) over the current 1.6 cell design working point (red diamond).

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Temporal Bunch Diagnostics

In collaboration with the group of Emilio Nanni, a THz time-tool method has been developed at MeV-UED using an optimized parallel-plate waveguide (PPWG) structure to couple THz radiation and provide a strong transverse momentum kick to the electrons [5]. The peak deflection observed corresponded to 150 MV/m of peak field at a pump energy of 7 mJ. The peak streaking achieved corresponds to a resolution of about 0.14 fs μrad^{-1} on the detector. Based on these initial analyses, we anticipate that with the implementation of a dedicated time-tool diagnostic combined with reduced bunch duration enabled by the proposed gun design, we can achieve 50 fs overall UED temporal resolution, compared with 150 fs in the current configuration. Implementing this technique for use in user experiments requires reconfiguration of the laser transport and a dedicated THz vacuum chamber and optical setup, which have been recently installed after the second sample chamber. The near-term goal is to implement the THz time-tool as a destructive diagnostic, to be upgraded to a fully online shot-to-shot measurement following upgrade of the ePix detector (now in progress) to include a through-hole for the electron beam. This approach will enable significantly improved temporal resolution for a range of ultrafast time-resolved pump-probe experiments by decoupling of the arrival time jitter between pump and probe pulses on a shot-to-shot basis.

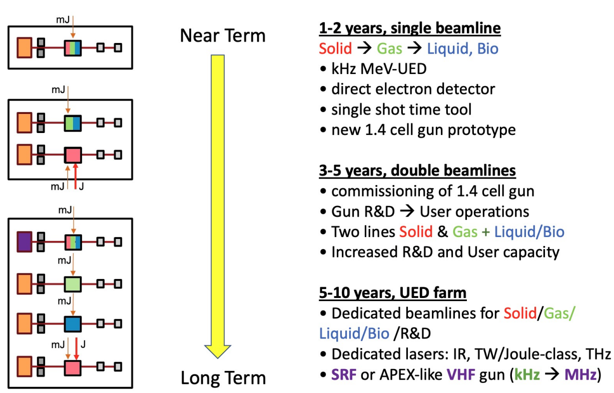

Figure 3: Envisioned Roadmap for future expansion and development of the UED instrument at SLAC.

LONG-RANGE OUTLOOK

The existing MeV-UED instrument is multi-purpose, with solid state, gas phase, and soon liquid-phase experiment capabilities on offer to users. However, due to the need to swap out instruments and chambers, a single beam line can only realistically accommodate one of these science areas per user run. Upgrades to the existing facility are limited in scope to improvements that are compatible with maintaining a rigorous experiment schedule with high scientific output. The current schedule of user experiments, R&D, and facility maintenance represents a maximal use of the existing single electron source delivery point. Extending substantially beyond this will require one or more additional beam lines operating in parallel with an appropriate diversification of measurement capabilities to better cover a broader array of science drivers. Commissioning of one additional beam line would afford invaluable opportunities to include more expansive capabilities that address the future needs outlined above. We view the above proposed R&D activities as the first step in a multi-phase development of the facility over a 5 to 10 year time scale, see Fig. 3, to include 1 to 2 additional beamlines to eventually form a "UED Farm" with diversified instrumentation and dedicated beam delivery capabilities. Incorporation of a superconducting or normal-conducting MHz rep rate RF gun on one or more of these beam lines would leverage ongoing development for LCLS-II-HE while enabling high probe rates with ultra-bright low emittance and low energy spread beams. Expansion of the MeV-UED facility will enable a new era of ultrafast pump-probe capabilities with ultra-bright electron beam and high-repetition-rate electron detector, providing a suite of powerful tools to address grand-challenge science in chemical and atomic and molecular optics.

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