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Utilising charge state distributions for calibration of intense XFEL pulses with Bayesian optimisation

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X-ray free-electron lasers (XFELs) provide a powerful tool to probe atomic and molecular dynamics with both exceptional temporal and spatial resolution. For a quantitative comparison between experimental results and their simulated theoretical counterpart, however, a precise characterisation of the X-ray pulse profile is essential. Generally, the pulse profile provides a non-uniform photon distribution that depends on space and time coordinates and hence, heavily affects the interaction between the X-ray pulse and the target. The determination of the pulse profile, referred to as calibration, constitutes a major experimental challenge and is yet inevitable.

Here, we propose a calibration scheme utilising charge state distributions (CSD) of light noble gas atoms. The corresponding experiments can be performed with little effort and, subsequently, be used for the calibration. In order to perform the pulse calibration, we employ high-level electronic structure simulations and a machine learning-based numerical optimisation technique called Bayesian optimisation (BO). The application of BO to experimental and theoretical data constitutes the main focus of our work.

We demonstrate that BO can accomplish the optimisation tasks efficiently and with high accuracy. We further show that the proposed calibration based on charge state distributions determines the spatial profile as well as the pulse duration of XFEL pulses with equivalent precision in comparison to a fully experimental determination. Therefore, the presented calibration scheme serves as a comprehensive, efficient, and accurate tool for XFEL pulse characterisation.

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