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Coulomb explosion as a high-dimensional probe of single molecules

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X-ray–induced Coulomb explosion imaging is one promising method to perform single-particle molecular imaging on a femtosecond timescale. By firing an intense ultrashort XFEL pulse at single molecules, it gets strongly ionized and violently dissociates into atomic fragments that are measured in coincidence. However, due to the finite detection efficiency in the experiment, the collected data is both unstructured and missing information, which precludes its analysis and interpretation. To get a coherent and informative picture of the data despite the challenges inherent to the experimental data, we developed a new analysis method inspired by machine learning techniques. We applied this methodology to the Coulomb explosion of 2-iodopyridine (C_5H_4NI), which allows us, in conjunction with simulations, to demonstrate that the experiment is measuring fingerprints of the collective nature of the quantum ground-state fluctuations of the molecule.

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