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Imaging collective quantum fluctuations of the structure of a complex molecule

Due to the Heisenberg uncertainty principle, the structure of a molecule fluctuates about its mean geometry, even in the ground state. Observing this fundamental quantum effect experimentally, particularly revealing the collective nature of the structural quantum fluctuations, remains an unmet challenge for complex molecules. We achieved this for an 11-atom molecule by inducing its Coulomb explosion with an x-ray free-electron laser. Relying on our simulations, we show that the structural fluctuations manifest themselves in correlated variations of ion momenta obtained via coincident detection of the atomic fragments from individual molecules. Then, a novel analysis scheme allows extracting these variations from the experimental data, despite measurements covering only a fraction of the full 33-dimensional momentum space, thereby establishing a general approach for extracting information on high-dimensional structural dynamics using Coulomb explosion.

Author: RICHARD, Benoît (CFEL-DESY, CUI)

Co-authors: Dr INHESTER, Ludger; Dr BOLL, Rebecca; SANTRA, Robin (CFEL, DESY); Prof. JAHNKE, Till

Presenter: RICHARD, Benoît (CFEL-DESY, CUI)

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