



Progress and remaining challenges in LIED, a "molecular selfie" technique

ICFO researchers review laser-induced electron diffraction (LIED), a high-resolution imaging technique that captures the structure of single gas-phase molecules using one of their own electrons, highlighting its main advantages and limitations.

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Molecules constantly evolve and interact with each other, adapting their structure accordingly in the process. One of the grand challenges in science is visualizing how molecules undergo these transformations. Ideally, scientists would like to pinpoint and track over time the location of all the atoms in a molecule. This is, however, an extremely demanding task. Achieving it would require technologies with extraordinary sensitivity to detect individual molecules and unparalleled precision to map their atoms in space and time. Laser-induced electron diffraction (LIED) makes imaging a single gas-phase molecule and locating all its atoms possible, achieving exceptional picometer (10⁻¹² meters) spatial and attosecond (10⁻¹⁸ seconds) temporal resolution. LIED has been extensively refined and successfully applied at ICFO, resulting in numerous impactful outcomes and highlighting the

institute's prominent role in driving progress in this state-of-the-art technique. ICFO researchers **Dr. Katharina Chirvi** and **ICREA Prof. Jens Biegert** have recently presented a comprehensive review of LIED in Structural Dynamics. In there, they give an overview of the technique, from its origins to the current state-of-the-art, explaining its underlying physical principles and focusing on the main strengths and limitations. **The article serves as a valuable resource for understanding the current state of LIED, its methodologies, and the future potential it offers for advancing molecular dynamics research.**

LIED's basic principles, strengths and weaknesses

The review explains the LIED's imaging process, which begins with a strong laser pulse focused onto a gas-phase molecule under study. The intense light ionizes the molecule liberating an electron that is initially driven away by the laser's electric field. In a phenomenon known as recollision, the electron reverses its trajectory and returns to scatter off its parent ion. This electron scattering generates a diffraction pattern that encodes information about the molecule's interatomic distances. By analysing this data, LIED reconstructs the molecule's 3D structure with picometer and attosecond resolution -pushing the boundaries of what is physically possible in imaging

Therefore **by employing one of the molecule's own electrons, the LIED technique achieves high-quality images**, which the authors refer to as *½molecular selfies½*. But this was not always the case. In its early stages, LIED could only image small linear and symmetric diatomic molecules. Over time, the technique evolved to retrieve 2D, and then also 3D molecular structures. Today, LIED can be applied to a variety of molecular systems, including large complex structures that were previously inaccessible. The article, though, emphasizes the importance of fulfilling several critical conditions for effective imaging, such as ensuring the electron has sufficient impact energy during recollision. The authors also describe different LIED implementations, each with its own set of advantages and limitations, which can also affect the overall performance and applicability of the technique. Looking ahead, the researchers highlight the importance of extending the temporal observation window available for the technique, something that *½would allow for a long-standing dream of scientists, namely, to produce atomic-resolution images of single molecules undergoing structural transformation½*

Reference:

Chirvi, J. Biegert; Laser-induced electron diffraction: Imaging of a single gas-phase molecular structure with one of its own electrons. Struct. Dyn. 1 July 2024; 11 (4): 041301.
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