

Wintersemester 2024-2025

Titel

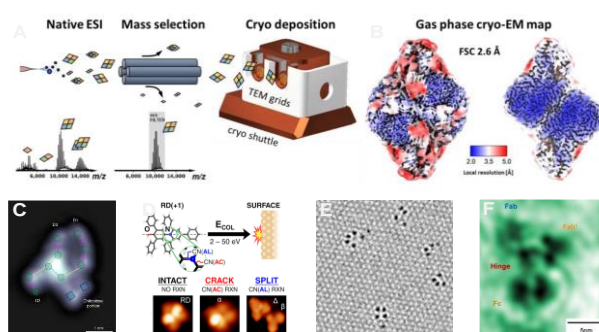
Atomic resolution molecular imaging by scanning probe and electron microscopy based on soft-landing electrospray ion beam deposition (ESIBD).

Vortragender

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Abstract

Electrospray ion beam deposition (ESIBD), the deposition of intact molecular ions created by electrospray ionisation onto solid surfaces in vacuum, has been introduced in our lab as a tool for the handling of large and complex, usually non-volatile molecules (see **Fig. A**).[1] Initially, the high-resolution single-molecule imaging by scanning probe microscopy (SPM) has been the major application. Here ESIBD proved successful in the investigation of structure, conformation, and properties of proteins, peptides, saccharides, and synthetic molecules (see **Fig. CD**).[2,3]



Molecular imaging based on ESIBD. (A) Scheme of native ESIBD deposition onto cryoEM grids.[1] (B) 3D density of b-gal prepared by native ESIBD.[5] (C) STM image of a branched 11-mer glycan.[2] (D) Hyperthermal chemistry: Intact Reichardt's Dye molecule and products of the hyperthermal collision in STM images. (E) Transmission electron microscopy of atomic clusters on freestanding graphene. (F) Low energy electron holography image of an antibody.

ESIBD's high level of control over molecular ion beam and environment opens new avenues in molecular imaging. Native ESI enables the chemically selective enrichment of folded proteins and proteins complexes for structural investigation by electron microscopy imaging (cryoEM)[4,5], and low energy electron holography (LEEH, **Fig. F**).

Optimized conditions for native deposition promote imaging of individual proteins at a resolution sufficient for the construction of atomic models from cryoEM data (see **Fig. B**).[5] The structure obtained from cryoEM after embedding the landed proteins in ice grown from the gas

phase shows a fold and subunit arrangement which is remarkably similar to the solution structure. Small conformational changes cause differences mostly at the protein surface and interfaces. We find the closing of cavities and crevices' due to self-interaction in absence of water, a change readily reversed in MD simulations to find the native solution structure.

References: [1] Rauschenbach, *Annu Rev Anal Chem* **9** (2016) 16.1-16.26. [2] Wu, *Nature* **582** (2020) 375-378. [3] Anggara, *Science* **382** (2023) 219-223. [4] Esser, *PNAS Nexus* **1** (2022) pgac153. [5] Esser, *Science Advances* **10** (2024) ead4628.

Ort

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Zeit

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gez. Professor Dr. Andreas Steffen

Gesellschaft Deutscher Chemiker Ortsverband Dortmund