



Contribution ID: 102

Type: **Talk**

Molecular signatures in the 3D- Δ -PDF

Tuesday, 15 March 2022 15:00 (20 minutes)

A systematic case study of the molecular signatures that can be observed in the 3D- Δ -PDF is presented. We will highlight the reason behind broad regions of negative 3D- Δ -PDF density and explain why situations arise in which intramolecular Patterson vectors are not observed in the 3D- Δ -PDF. In combination with current advances in initial data processing we will lay out the basis for a systematic 3D- Δ -PDF atlas.

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Session Classification: Advanced Structure Analysis II

Track Classification: Main conference: Advances in Methods, Instrumentation and Data Analysis