Oral presentation

# PXRD-Assisted Crystal Structure Predictions

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Crystal structure prediction (CSP) algorithms serve as indispensable tools for determining stable and metastable phases associated with specific chemical compositions [1]. Despite their utility in structural recognition from experimental data, particularly in powder X-ray diffraction (PXRD), discrepancies between predicted and experimental results persist, especially under compression. These disparities stem from various factors such as computational approximations (*e.g.*, choice of level of theory, pseudopotential, and the assumption of 0 K conditions) and experimental conditions (*e.g.*, high-pressure) [2]. Consequently, achieving optimal matches with experimental data often entails screening numerous metastable phases, posing challenges, especially in polymorphic systems with minimal energy differences.

To address this challenge and potentially improve matching accuracy, biasing CSP algorithms offer a promising solution. Herein, we present our approach to enhancing crystal structure predictions by integrating PXRD data in the CSP software XtalOpt [3]. Leveraging XtalOpt's multi-objective search capability [4], we expedite structural recognition of PXRD patterns collected at ambient and non-ambient conditions, particularly beneficial when the experimental PXRD diverges from the computational ground state phase but aligns with a metastable or distorted structures. This acceleration is achieved through the integration of PXRD similarity modules implemented into XtalOpt's crystal structure search.

Our methodology offers a systematic framework for incorporating experimental data into CSP algorithms (Figure 1) [3], thereby improving the efficiency and accuracy of crystal structure predictions and facilitating advancements in materials and planetary science.

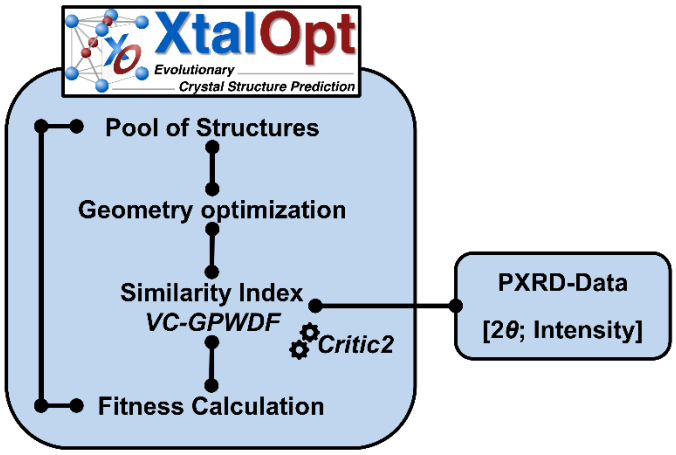


**Figure 1**. Workflow of a PXRD-assisted crystal structure prediction[3].

[1] E. Zurek, in *Handb. Solid State Chem.*, Wiley-VCH Verlag GmbH & Co. KGaA, **2017**, pp. 571–605.

[2] M. A. Neumann, F. J. J. Leusen, J. Kendrick, *Angew. Chemie - Int. Ed.* **2008**, *47*, 2427–2430.

[3] S. Racioppi, D. la Roza, A. Otero, S. Hajinazar, E. Zurek, *arXiv Prepr.* **2024**, arXiv:2407.05394.

[4] S. Hajinazar, E. Zurek, *Comput. Phys. Commun.* **2024**, *304*, 109306.