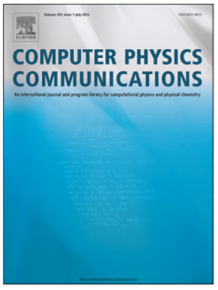

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X-ray diffraction data-assisted structure searches

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X-ray diffraction (XRD) is an important technique for structure determination. However, in traditional methods, estimated structural information (e.g., unit cell parameters and space group) is required to determine the precise structure from XRD data. We propose a versatile global search method for determining crystal structures from experimental powder XRD data without guessed structural information. Unlike in traditional structure prediction, which uses total energy as the fitness function, the fitness in our method is the degree of dissimilarity between the simulated and the experimental XRD patterns. To improve the efficiency of structure searching using powder XRD data, several techniques are implemented, including background subtraction, profile parameter optimization by simulated annealing, and structure evolution using CALYPSO. The efficiency and robustness of our method is demonstrated here using predictions of previous known structures (hexagonal ZnO and anatase TiO_2). The method is also used to explore the high-pressure phases of binary compounds $CaLi_2$ and Ca_3C_2; it uncovers candidate structures ($C222_1$ for $CaLi_2$ at 54 GPa and $Cm2m$ for Ca_3C_2 at 12.5 GPa) whose simulated XRD patterns agree with their experimental patterns.