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Implementation of a methodology for crystal structure prediction using genetic algorithms integrated into the Python ASE library

Thursday, 12 June 2025 16:00 (20 minutes)

This talk is dedicated to the development and implementation of a methodology for crystal structure prediction using genetic algorithms integrated into the Python ASE library.

The application of genetic algorithms for crystal structure prediction holds great potential in various fields, particularly in materials science and nanotechnology.

The main objective is to develop an efficient tool that enables automation and acceleration of the process of finding optimal crystal structures for specific applications.

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