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CrysFieldExplorer: Rapid Optimization of the Crystal Field Hamiltonian

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We present a new approach to the fast optimization of crystal electric field (CEF) parameters to fit experimental data. This approach is implemented in a lightweight Python-based program, CrysFieldExplorer, using Particle-Swarm-Optimization (PSO) and covariance matrix adaptation evolution strategy (CMA-ES). The main novelty of the method is the development of a unique loss function, referred to as the spectrum characteristic loss, which is based on the characteristic polynomial of the Hamiltonian matrix. Furthermore, this optimization technique can be generalized to optimize spin wave excitations by performing optimization on multiple exchange Hamiltonian matrices at multiple Q positions in reciprocal space.

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