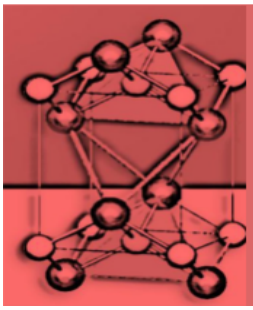

IX Workshop on Novel Methods for Electronic Structure Calculations

10th – 19th November 2021
La Plata – Argentina

Calculating 4f Crystal-Field States by Density Functional Theory

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This lecture provides an overview of existing methods to determine the parameters of a 4f single-ion model by meansof density functional theory (DFT). The standard model of 4f magnetism is introduced, justified, and explained. The ingredients to evaluate its parameters (exchange field and crystal field) are the radial 4f wave function, constructed under observation of the localized character of 4f states, and an appropriately constrained Kohn-Sham potential. Three different implementations of crystal-field parameters from DFT are presented and discussed, and four methods beyond the single-ion model are evaluated.