

Self-interaction correction calculations of f-electron materials

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The self-interaction corrected local spin density (SIC-LSD) approximation is reviewed. This scheme allows for a localized description of some of the electronic degrees of freedom, and the self-interaction energy acts as an energy of localization which conquers the energy gained upon band formation. Applications to f-electron materials are discussed with emphasis on systems with competing valencies, notably SmS, TmSe and PuSe. In particular, PuSe is seen as equivalent to SmS under compression. While cohesive properties of localized systems is generally well described by SIC-LSD, other aspects of the electronic structure need further modelling. The atomic-like multiplet structure of the excited states is one prominent example. The photoemission spectra of f-electron compounds are modelled by a dynamical mean field theory. The complete multiplet spectrum of a single ion is calculated by exact diagonalization of the two-body Hamiltonian of the f^n shell, and the ensuing atomic self-energy operator is combined with the LDA Hamiltonian. For PuSe, additional interaction between the Pu f -shell and the conduction electrons must be incorporated.