First-principles Investigation on the Electronic Structures and Magnetic Properties; Using All-electron FLAPW Method

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We’re witnessing the golden age of innovation with novel materials in both basic science and technological point of view, where the computation and simulation are playing an important role as a major component. The first-principles electronic structure investigation is one of the crucial parts of the computational material science. In this talk, we’re going to review and discuss the all-electron approach of the DFT based electronic structure investigations from the basics to the specific advances including the various spin-orbit coupling induced phenomena.