

A unified approach to physical properties of complex solids

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Physical properties induced by exchange interactions (Curie temperature and spin stiffness) and spin-orbit coupling (residual resistivity, anomalous Hall effect, anisotropic magneto-resistance, and Gilbert damping) are determined from a unified electronic structure model (the Green-function formulation of the tight-binding linear-muffin tin orbital approach) in which the effect of possible disorder is included in the framework of the coherent-potential approximation.

The first-principles Liechtenstein mapping generalized to random alloys is employed to construct the effective Heisenberg Hamiltonian and to estimate Curie temperature and spin stiffness in framework of the real-space random-phase approximation.

Recently developed Kubo-Bastin transport theory and nonlocal torque operator formulation of the Gilbert damping are used to determine above mentioned transport properties and damping coefficients. As a case study we employ diluted (Ga,Mn)As ferromagnetic semiconductor alloys.

Good agreement of calculated physical quantities with experiments on well-annealed samples containing a small amount of compensating defects is obtained.