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Orbital Polarization in Itinerant Magnets IGOR SOLOVYEV, National Institute for Materials Science, Tsukuba, Japan — The correct description of the orbital magnetism is one of the longstanding problems in the density functional theory (DFT). One possible solution is to extend DFT by considering explicit dependence of the exchange-correlation energy on the orbital degrees of freedom. Since the angular momentum operator does not commute with electrostatic potential, it is not an observable except a small atomic region where this potential is nearly spherical. Hence, the orbital magnetism is an atomic property, and we inevitably have to deal with the problem of on-site Coulomb interactions and screening of these interactions in solids.[1] For itinerant systems, this screening can be evaluated in the random-phase approximation (RPA), by considering the strong-coupling limit. Then, the orbital polarization can be computed as the self-energy correction in the static version of the GW method, without any adjustable parameters.[2] This opens a formal way for combining the spin itineracy in the local-spin-density approximation (LSDA) with the atomic orbital magnetism. RPA can be further improved by restoring the spin polarization of LSDA through the local- field corrections. Numerical applications reveal a remarkable improvement for the orbital magnetization and magnetocrystalline anisotropy energies of transition metals and actinide compounds. [1] I. V. Solovyev *et al.*, Phys. Rev. Lett. **80**, 5758 (1998). [2] I. V. Solovyev, Phys. Rev. Lett. **95**, 267205 (2005).

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