

# Density functional calculations of the magnetic structure of FePt nanoparticles

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The spin moment distribution in magnetic nano-particles is both scientifically interesting and technologically relevant. Here, we present the magnetic structure of FePt nano-particles, as determined by projector-augmented wave (PAW) and locally self-consistent multiple scattering (LSMS) local density calculations on nano-particles up to 3nm in size. The magnetic structure changes as a function of nano-particle size, composition, and chemical order, encompassing both ferromagnetic and anti-ferromagnetic tendencies. This behavior will be described and related to charge redistribution, structural relaxation, and local coordination.

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