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Enhancing Inter-phase Exchange Coupling in $SmCo_5$/Co Nanocomposite Materials[1] DANGXIN WU, QIMING ZHANG, J.P. LIU, University of Texas at Arlington — Exchange-coupled hard/soft phase nanocomposite magnets were proposed to increase the maximum energy product by combining the large anisotropy of hard phase materials and the high saturation magnetization of soft phase materials. To understand the inter-phase exchange coupling is very important for design of nanocomposite magnets. In this work, we performed first-principles calculations to investigate the inter-phase exchange coupling between hard phase $SmCo_5$ and soft phase Co using superlattice model. The calculations were based on Density Functional Theory, using projector augmented wave (PAW) method and linear-muffin-tin-orbital (LMTO) method in the atomic sphere approximation. The atomic structures were optimized and the electronic ground state was obtained. Then the noncollinear magnetic calculations were performed to calculate the exchange interactions. We found that the total energy is a quadratic function of angle (θ) between the directions of magnetic moments of hard phase and middle layer of soft phase. We found that Fe doped soft phase strengths the exchange coupling between $SmCo_5$/Co in our models, which in turn may lead to higher maximum energy product.

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