

Abstract Submitted
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First-principles study of interface exchange coupling in SmCo₅/Co nanocomposite materials¹ DANGXIN WU, QIMING ZHANG, J.P. LIU, University of Texas at Arlington, RENAT F. SABIRIANOV, University of Nebraska-Omaha — Understanding the interface exchange coupling is very important in designing and enhancing the performance of exchange-coupled hard/soft phase nanocomposite magnets, which 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. In this talk, we will present our results of our recent first-principles calculations in investigate the interface exchange coupling between hard phase SmCo₅ and soft phase Co using superlattice model. The calculations were based on Density Functional Theory. The atomic structures were optimized and the electronic ground state was obtained. Then the noncollinear magnetic order calculations were performed to study the exchange interactions. We found that the change of 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 also performed calculations on a SmCo₅/CoFe system in which the soft phase was doped with Fe. Comparison and discussions will be made between these two systems.

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