Computational design high-performance rare-earth-free permanent magnet based on hard-soft hybrid structures

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Permanent magnets (PMs) are playing a key role in modern industry, particularly in energy conversion applications, mostly mechanical to electrical or vice versa, which includes automobiles, electronics and power generators. The conversion efficiency of such devices critically depends on the magnets' performance, which makes it a first-priority task to develop PMs with higher strength. Today, most high-performance magnets are based on rare-earth elements such as Nd, Sm or Dy. Going through the so-called "Rare-earth crisis" around 2010, many countries initiated interdisciplinary research programs to design novel PMs without containing rare-earth elements. In this talk, we will present our recent results along this direction using the exchange spring magnet. By employing first-principles density functional theory, we compute important magnetic properties for strong PMs, saturation magnetization (M_s), energy product ($(BH)_{max}$) and coercivity (H_c), of hard-soft hybrid structures which consist of periodic arrangement of MnBi and Fe layers. Through calculating the magnetic properties by varying the thickness of each phase, we demonstrate that M_s, $(BH)_{max}$ and H_c of MnBi/Fe all show large improvement over MnBi; Compared to MnBi, M_s, $(BH)_{max}$ and H_c of the hybrid structure are increased by 20%, a factor of two and three, respectively. These findings indicate that MnBi/Fe holds a great potential for high-performance, rare-earth-free permanent magnet for next-generation applications.