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Understanding magnetism in transition-metal multilayer thin-films on MgO(001) by using machine-learning technique K. NAKAMURA, K. NOZAKI, Mie University, K. HUKUSHIMA, The University of Tokyo, H. KINO, National Institute for Materials Science, T. AKIYAMA, T. ITO, Mie University, T. OGUCHI, Osaka University — New computational approaches for exploring materials with many exciting properties continue to grow in modern material science. In the field of spin-electronics, however, the effective procedure is still lacking due to a difficulty in treating magnetism, while searching promising ferromagnetic transition-metal (TM) multilayer thin-films with large perpendicular magnetocrystalline anisotropy (MCA) is strongly desired, e.g., for successful magnetic tunnel junction devices. Here, in order to show the underlying trends and physics in the magnetism in multilayer thin-film systems, we carried out first principles calculations by employing six-atomic-layer slabs of Fe and Au (Co and Au) on MgO(001). With an assist of the cluster-expansion method, the magnetic moments are found to follow the Slater-Pauling rule, i.e., governed by composition of the constituent TMs. In contrast, the MCA energy dramatically depends on the atomic-layer alignments with very large variation up to 5 meV/atom-area from a negative value of -2 meV/atom-area. Compressing sensing for understanding such dispersive MCA will be further applied.

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