Magnetic anisotropy and magnetoelectric effect in 3d transition metal systems

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Abstract: Spintronics has drawn lots of attention from the science community due to its advantages compared with traditional charge-based electronics arising from using the electron spin to carry information. By adding the spin degree of freedom to electronics, the new spintronics devices would be non-volatile, have high data processing speed but low electric power consumption. However, before successful application of spintronics, there are two basic issues, one is how to "store" spin and the other is how to manipulate spin. For the former issue, magnetic anisotropy energy is the crucial parameter which determines the capability of magnetic systems to resist thermal fluctuations and quantization effects. Thus, it is significant to find magnetic systems with large magnetic anisotropy energy. Regarding to second one, the best way is to manipulate spin by electric fields. In this case, the spintronic devices are more convenient to integrate to modern semiconductor circulars. In this talk, I will discuss the magnetic anisotropy of single Co atom on MgO monolayer and the magnetoelectric effect of Co doped ZnO and TiO₂. Based on first-principles calculations, we provided an insight to understand the origin of large magnetic anisotropy and predicted a possible way to achieve electrically controllable spin direction.

