

## **Effects of strain, gas adsorption, and capping on magnetocrystalline anisotropy of Co(0001) and Fe(001) surfaces: A first-principles study**

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Intense scientific efforts to increase information density in devices such as magnetic-resistance access memory (MRAM) have been paid during last few decades. Recently, so-called spin transfer torque random access memory (STT-RAM) has been emerged in a nano-scaled magnetic tunnel junction (MTJ) with advantages of good selectivity in writing, low power consumption, and high scalability over conventional MRAM. Two key factors of (1) high thermal stability and (2) low critical current density for switching of magnetization orientation should be satisfied to realize commercialized STT-RAM. An MTJ with strong perpendicular magnetocrystalline anisotropy (PMCA) is indispensable for the two key factors [1]. In this talk, some suggestions will be given to enhance MCAs of the typical magnetic systems of Co(0001) and Fe(001) surfaces, based on our first-principles studies on effects of strain, gas adsorption, capping of 4d/5d transition metal on the MCAs. Physical origins will be discussed in terms of single particle energy spectra.

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[1] J. Z. Sun, Phys. Rev. B 62, 570 (2000).