**A first-principles study on the magnetism of**

**Fe/Bi/MgO multilayers**

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The magnetic tunnel junction (MTJ) has a structure consisting of two ferromagnetic layers separated by a thin insulating layer. MTJ is used for the magnetoresistive random access memory (MRAM) cell with giant magneto resistance ratio. MRAM is a nonvolatile memory without requiring standby power to keep information and has attracted much attention as a new generation of low power consumption memory. Strong perpendicular magnetic anisotropy to realize high density memory devices is highy desired for preventing thermal magnetic fluctuation in the ferromagnetic layer of MTJ. Perpendicular magnetic anisotropy originates from magnetocrystalline anisotropy (MCA) caused by spin-orbit coupling. In this study, we investigate the influence of a Bi layer insertion at Fe/MgO interface by first-principles density-functional calculations. We first propose models of Fe/Bi/MgO by considering lattice matching for the calculations and then study the magnetism of Fe/Bi/MgO as well as Fe monolayer and Fe/MgO films. It is found that enhancement in perpendicular magnetic anisotropy can be obtained by inserting the Bi layer at the Fe/MgO interface. The electronic origin of MCA in the systems is discussed from the viewpoint of Bruno’s formula [1] and band structure within the second-order purturbation theory [2].

[1] P. Bruno, Phys. Rev. B **39**, 865 (1989).

[2] D. S. Wang, R. Wu, and A. J. Freeman, Phys. Rev. B **47**, 14 932 (1993).