

# Magnetolectric effect of strained 5d TM/Fe/MgO(001) (TM=Ta and Pt): A first principles study

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Electric field effect on magnetization and magnetocrystalline anisotropy (MCA) of strained 5d TM/Fe/MgO(001) [TM=Ta and Pt] has been investigated using first-principles calculations. Up to the 4% compressed strain with respect to MgO substrate, the Ta/Fe/MgO(001) always exhibits PMCA, while MCA of Pt/Fe/MgO(001) is switched from in-plane MCA of -2.18 meV/cell (without strain) to PMCA of +0.74 meV/cell (under 4% compressed strain). Moreover, the magnetolectric effect is studied under the electric field perpendicular to the surface. For Pt/Fe/MgO, the PMCA is enhanced to +1.09 meV/cell ( $E=+1$  V/Å), while decreased to +0.03 meV/cell ( $E=-1$  V/Å) in Fig 1. Further, we will discuss origin of magnetolectric effect at the interface of 5d TM/Fe/MgO(001).

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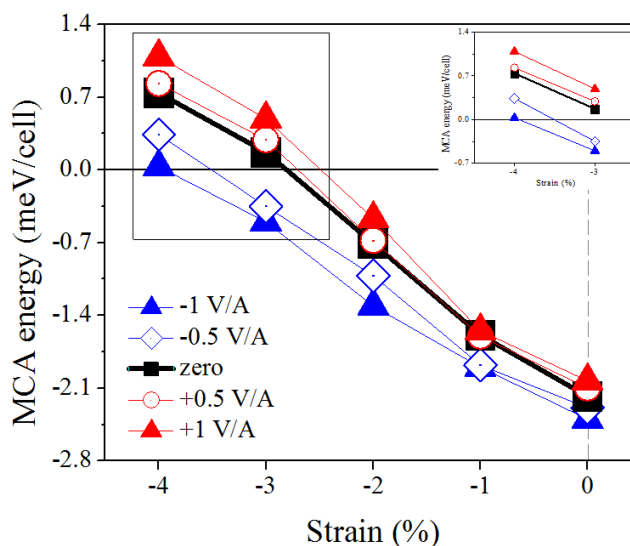


Fig 1. Electric field effect on MCA of strained Pt/Fe/MgO.