First Principles Insights into Spintronic and Spin-Orbitronic Phenomena in Magnetic Nanostructures

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Ab initio insights are provided into spin-orbit coupling based phenomena such as perpendicular magnetic anisotropy (PMA) [1-6] and Dzyaloshinskii-Moriya interaction (DMI) [7-10] at interfaces comprising transition metals, insulators, or graphene. First, the nature of PMA at Fe|MgO interfaces is unveiled by evaluating orbital and layer resolved contributions to PMA in Fe/MgO interfaces and MTJs with different interfacial conditions [1-3] (Fig. 1). Mechanisms of the optimization of effective anisotropy as well as of its electric field control are discussed [4-6]. Next, the main features and microscopic mechanisms of DMI behavior are elucidated in Co/Pt and other Co/heavy metal bilayers [7,8] (Figs. 2-4). Furthermore, several approaches for DMI enhancement and manipulation will be presented including, in particular, physical mechanisms of DMI behavior in Pt/Co/MgO structures [8,9] allowing observation of room temperature skyrmions [9]. The behavior of PMA and DMI will then be addressed for nanostructures comprising Co/graphene interfaces [10,11] (Figs. 5,6) which may be of strong interest for graphene spintronics [12,13].

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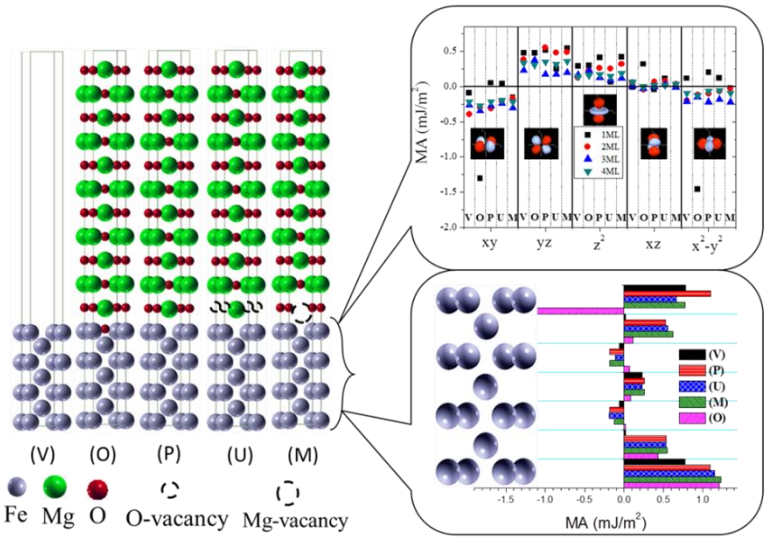

Fig.1: Layer- and orbital-resolved anisotropy contributions for crystalline structures: (V) Fe/vacuum, (O) overoxidized Fe7/MgO, (P) pure Fe7/MgO11, (U) underoxidized Fe7/MgO, and (M) Mg vacancy in Fe7/MgO11. From Refs. [1,3].

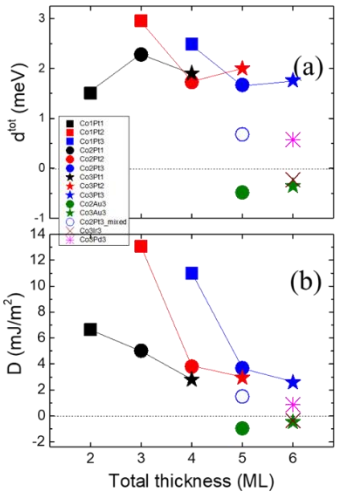

Fig.2: (a) Microscopic (d^{tot}) and (b) Micromagnetic (D) DMI coefficients for the Co/Pt, Co/Ir, Co/Au, Co/Pd bilayers as a function of the total number of atomic layers.

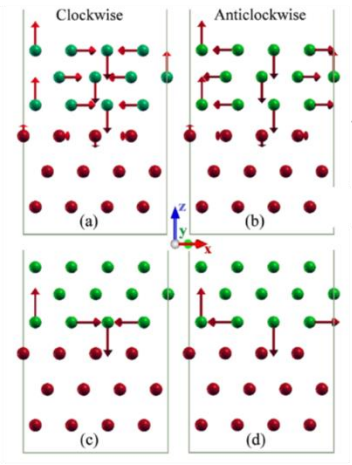

Fig.3: Examples of (a),(c) clockwise (CW) and (b),(d) anticlockwise (ACW) spin configurations to calculate the DMI hcp(0001)Co/fcc(111)Pt bilayers. Green and red correspond to Co and Pt.

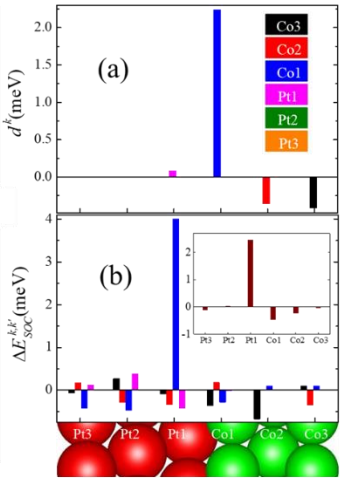

Fig.4: (a) Layer resolved DMI coefficient d^k vs layer k and (b) the corresponding localization of the associated SOC energy source in the atomic sites of all layers k'.From Ref. [7]

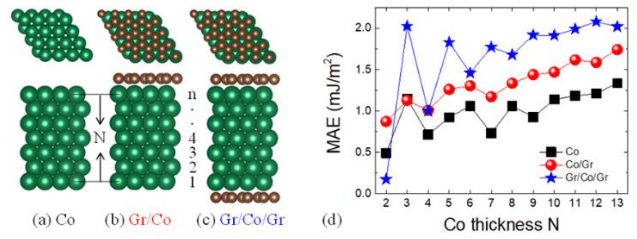

Fig.5: Top and side view of (a) bare Co slab, (b) Co on graphene, and (c) Gr/Co/Gr, respectively. (d) Magnetocrystalline anisotropy energy as a function of Co thickness N (monolayers).

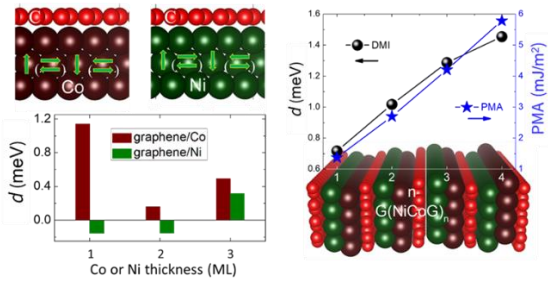

Fig.6: Top- and side-view of graphene on a hcp Co(0001) and on a fcc Ni(111) surfaces. DMI coefficient as a function of Co(Ni) thickness. DMI and PMA for multilayers of graphene/[Co/Ni/graphene]$_n$ as a function n.