MRAM at the Atomic Edge: The Search for Magnetic 2D materials

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While spin-transfer-torque MRAM devices are now commercially available, there are still significant challenges (device size, power consumption, reliability) that must be addressed to move this technology to a broader market. Optimizing materials and interfaces in these structures can help in solving many of these issues. However, the wide material parameter space makes this a difficult problem to tackle from a purely experimental Edisonian approach. The dilemma highlights the need for improved theoretical insight coupled with the ability to rapidly perform broad material searches. The recent emergence of cheap high performance computers coupled with efficient numerical algorithms has led to nimble simulation tools that can provide atomistic insight into key materials and interfaces for magnetic memory applications. Industry is increasingly relying on these approaches to help guide decisions in materials composition and interface engineering for next generation devices.

In this talk, I will provide a brief overview of the simulation effort at Western Digital and discuss some of our work focused on optimizing interfacial and film properties for spin-orbit-torque assisted MRAM. Following this, I will discuss the potential benefits and possible challenges of shrinking MRAM devices to the atomic limit by integrating 2D materials into the device stack. As one promising example, I will highlight my recent collaboration with Prof. Richard Hennig's group (University of Florida) that centered on identifying intrinsic two dimensional half metals [1]. Fully spin polarized metals have long been sought out in the magnetism field as an ideal electrode for fully spin polarized currents and high magnetoresistance devices. Numerous groups have focused on using half metal Heusler alloys for high spin polarization. However, in practice, these alloys often suffer from disorder and strain effects during deposition and processing that limit their effectiveness [2]. A 2D half metal analogue could offer key advantages due to the general lack of defects and dangling bonds and also given that van der Waals interactions may help minimize the impact of interfaces on the half metal character. To rapidly identify potential half metals, we performed a broad search of over 600 2D materials available in the MaterialsWeb repository [3]. All 2D materials were first evaluated using density functional theory at the PBE exchange-correlation level. For 30 promising half metal candidates, the energy difference between ferromagnetic and antiferromagnetic configurations was then considered. This led to 20 final candidates which were further investigated using the HSE06 hybrid functional. Out of these, only the three iron dihalides ($FeCl_2$, $FeBr_2$, FeI_2) in the 1T structure remained half metallic. I will discuss the magnetic properties of these interesting 2D materials, the potential and challenges for isolating the atomic films and integrating them into devices, and how their properties relate to their bulk layered metamagnetic cousins.

[1] M. Ashton et al., Nano Letters, **17,** 5251 (2017).

[2] M. R. Page et al., J. Appl. Phys., **119**, 153903 (2016).

[3] MaterialsWeb 2D materials repository https://materialsweb.org