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Modern computational magnetism: role of noncollinear magnetis in complex magentic phenomena

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Significant progress has been achieved from advanced first-principles FLAPW[1] calculations for the predictions of surface/interface magnetism such as enhanced magnetic moments and magnetic phenomena induced by the spin-orbit coupling (SOC) – and most recently by providing new predictions and understanding of magnetism in novel materials such as magnetic semiconductors. However, one unresolved challenging issue remains – the role of non-collinear magnetism (NCM) that arises not only through the SOC but also from the breaking of symmetry at surfaces and interfaces. This talk describes some recent developments in the theoretical/computational description of complex magnetic phenomena based on our newly developed generalization of our bulk[2] and film[1] (single slab) FLAPW methods to treat noncollinear magnetism (NCM) with no shape approximation for the magnetization[3,4]. As presented here, this approach has proven highly successful in describing complex magnetic phenomena such as perpendicular MCA in transition metal overlayers and superlattices; unidirectional anisotropy and exchange bias in FM and AFM bilayers; constricted domain walls important in quantum spin interfaces; and curling magnetic nano-scale dots as new candidates for non-volatile memory applications.

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