New insights on the Dzyaloshinskii-Moriya interaction

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We have derived an expression of the Dzyaloshinskii-Moriya interaction (DMI), where all the three components of the DMI vector can be calculated independently, for a general, non-collinear magnetic configuration. The formalism is implemented in a real space – linear muffin-tin orbital – atomic sphere approximation (RS-LMTO-ASA) method. We have tested our implementation for systems such as Mn_3Sn, trimers Cr on Au(111) and Mn on Ag(111) and Au(111); as well as Mn dimer on W(001). Our results have shown that non-collinear magnetism changes drastically the values and directions of the DMI and differently from the conventional DMI, that discrepancy does not come directly as a spin-orbit coupling effect. We give a macroscopic explanation to this by dividing the DMI into spin- and charge-currents contribution and studying the relation between the non-collinearity and the emergence of these currents. For the dimer case, we explicitly show the part of the DMI that comes from the spin-orbit coupling and the part of the DMI that comes from the non-collinearity. It highly suggests that, in small clusters, high-order of DMI-like terms in the spin-Hamiltonian become strongly relevant, e.g. four-spin, six-spin interactions. We believe that these results are important in the study of excited states of small clusters and its spin-dynamics.