Magnetic state transitions of Mn dimer on carbon-doped h-BN surface through external electric field

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Abstract
Using density functional theory we first show that the interaction between two Mn atoms can be tuned from antiferromagnetic (AFM) to ferromagnetic (FM) state by creating charge disproportion between the two atoms by customizing the ligands. The non-metallic planar heterostructures designed by doping carbon atoms in h-BN sheet are considered as the substrates for Mn dimer to study the magnetic properties. This 2D platform is introduced to design a model analogous to the triatomic cluster to manipulate the charge transfer from the Mn dimer to switch the magnetic states. External electric field is applied normal to the plane of substrate to control the charge transfer between Mn atoms and the surface. Depending upon the concentration of carbon in h-BN sheet and strength and direction of applied electric field, magnetic states of the dimer can be switched from AFM to FM and vice versa. Using these two magnetic states (FM and AFM) one can store one-bit (0 or 1) information per chip.

Magnetic transition of Mn dimer

Equilibrium geometrical structures of Mn$_2$ and Mn$_2$X (X = H, Cl) clusters

Mn dimer adsorbed on C-doped h-BN monolayer of 8x8 supercell.

C-doped h-BN

Electronic band structures of h-BN and C-doped h-BN structures

Relative energy difference of various orientation of Mn$_2$ dimer placed on h-BN and C-doped h-BN substrate with respect to stable configurations.

Conclusions
- The magnetic states of the dimer can be tuned by changing the doping concentrations of carbon in h-BN monolayer as well as applying electric field normal to plane of substrate.
- The underlying origin of switching of magnetic states viz. FM to AFM and vice versa is the result from charge transfer between Mn dimer and the substrates.