

## Inter-IISER Chemistry Meet (IICM 2017)

### Emergence of Ferromagnetism at the interface of LaAlO<sub>3</sub>|CaMnO<sub>3</sub>: Non Magnetic Band and Mott Insulator

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#### Abstract:

Interface engineering has been used to create oxide heterostructures resulting in material systems with emergence of novel properties. New properties are results of complex interplay of various interactions at the interface originating from electronic and lattice degrees of freedom. This approach has been exploited to experimentally synthesize superlattices and oxide heterostructures such as CaRuO<sub>3</sub>/CaMnO<sub>3</sub>[1] and LaAlO<sub>3</sub>/SrTiO<sub>3</sub>[2] where interfacial ferromagnetism and metallicity emerge despite these properties being absent in the component materials. These discoveries have led to novel physics as well as interesting possibilities for applications.

In the present work, we investigate the electronic properties of a new oxide heterostructure formed with LaAlO<sub>3</sub> and CaMnO<sub>3</sub>, a band and a Mott insulator respectively. Our calculations employing a DFT + U approach find emergence of ferromagnetism and metallicity at the interface which is surprising since neither property is present in the component oxides. The magnetisation extends up to two layers into CaMnO<sub>3</sub> in contrast to what has been suggested in experiments in other related systems.

#### References

[1] He, C. ; Grutter, A. J.; Gu, M.; Browning, N. D.; Takamura, Y.; Kirby, B. J.; Borchers, J. A.; Kim, J. W.; Fitzsimmons, M. R.; Zhai, X.; Mehta, V. V.; Wong, F. J.; Suzuki, Y; *Phys. Rev. Lett.* 2012, 109, 197202.

[2] Fitzsimmons, M. R. ; Hengartner, N. W. ; Singh, S. ; Zhernenkov, M. ; Bruno, F. Y. ; Santamaria, J. ; Brinkman, A. ; Huijben, M. ; Molegraaf, H. J. A. ; Venta, J. de la; Schuller, Ivan K.; *Phys. Rev. Lett.* 2011, 107, 217201