MS19-01 | Orbital Molecules in Oxides

Attfield, J. Paul (University of Edinburgh, Edinburgh, GBR)

Orbital molecules are weakly bonded clusters of transition metal ions within an orbitally ordered solid [1]. The importance of these quantum states has become apparent in recent years following the discovery of 'trimeron' orbital molecules in the ground state of magnetite (Fe_3O_4) [2]. Determination of the full superstructure below the famous Verwey transition at 125 K showed that Fe^{2+}/Fe^{3+} charge ordering occurs with a pronounced orbital ordering of Fe^{2+} states that leads to localization of electrons in the linear, three-Fe trimerons. Recent results on orbital molecule orders in doped magnetites including natural samples will be presented [3]. Vanadium oxides also provide many examples of orbital molecule orders, associated with NTE (negative thermal expansion) in the orbital polymer material V_2OPO_4.[4] Persistence of large orbital molecules to high temperatures is discovered in the spinels AlV_2O_4 [5] and the new analog GaV_2O_4 [6]. Electronic phase separation driven by trimeron formation has recently been reported in $CaFe_3O_5$ [7]. Finally, some recent results revealing the origin of the Verwey transition will be presented [8]

[1] J. P. Attfield, *APL Materials* 2015, **3**, 041510.
[2] M.S. Senn, J.P. Wright, J.P. Attfield, *Nature* 2012, **481**, 173.
[3] G. Perversi, et al, *Chem. Comm.* 2016, **52**, 4864.
[4] E. Pachoud,et al, *J. Am. Chem. Soc.* 2018, **140**, 636.
[5] A. J. Browne; et al. *Phys Rev Mat* 2017, **1**, 052003.
[6] A. J. Browne; et al. *Inorg. Chem.* 2018, **57**, 2815.
[7] K. H. Hong, et al *Nature Comm.* 2018, **9**, 2975.
[8] G. Perversi, et al, submitted.