MS22-01 | 'PANCAKE' BONDING - A CHARGE DENSITY PERSPECTIVE

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The 1,2,3,5-dithiadiazolyls (R-CNSSN$^{\bullet}$, hereafter DTDAs), a family of thiazyl radicals, have been the focus of much investigation due to their potential as building blocks for magnetic and conducting materials. [1] However, these molecules tend to dimerise in the solid state *via* a spin-pairing interaction known as 'pancake bonding', a two-electron multi-centre interaction between π-radicals [2]. This dimerization renders the resulting materials diamagnetic. Much effort has been devoted to overcoming this interaction to produce magnetic materials.

In order to gain a deeper understanding of pancake bonding, experimental charge density analysis has been carried out on a number of DTDA homodimers, heterodimers and monomers. [3] These data, as well as various computational results, are assessed to probe the nature of the pancake bonds in DTDAs.

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