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Application of Charge & Band-flipping to Time-of-Flight Neutron Diffraction Data

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Charge-flipping has become a popular approach to ab-initio structure solution from X-ray powder diffraction data in particular due to its speed and need for minimal input other than lattice parameters. Given the appetite of charge-flipping for low d-spacing reflections, time-of-flight (TOF) neutron data should be a good match from a resolution standpoint, with easy access to high Q and lack of form-factor drop-off. One obvious issue with neutron data is the presence of elements with negative scattering lengths, where the inherent assumption of atoms always having positive 'density' in the algorithm breaks down. This means that portions of the structure can be effectively invisible. Given that some of these elements (e.g. H and Mn) are commonly found in samples of interest the issue is more than simple academic curiosity. Of course such atoms can be found by difference maps, but the issue has also been addressed within the charge-flipping algorithm with the 'band-flipping' modification [1]. Although Oszlányi & Sütő demonstrated the approach was viable with simulated neutron single crystal data [1], to the authors' knowledge it hasn't been used previously with experimental single crystal or powder neutron diffraction data. Powder diffraction data from POWGEN and wavelength-resolved TOF Laue single crystal data from TOPAZ at the Spallation Neutron Source have been used to probe the relative ease of charge-flipping with different TOF data using the TOPAS software package [2]. In addition the effectiveness of different customized band-flipping approaches has been tested to extract positions for positive and negative scattering elements simultaneously.

[1] G. Oszlányi, A. Sütő, *Acta Cryst.*, 2007, A63, 156-153, [2] A. Coehlo, "TOPAS Academic", version 5, Brisbane, Australia, 2014

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