Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Theoretical and experimental investigation on structural, electronic and magnetic properties of layered Mn_5O_8

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1 Supplementary Information

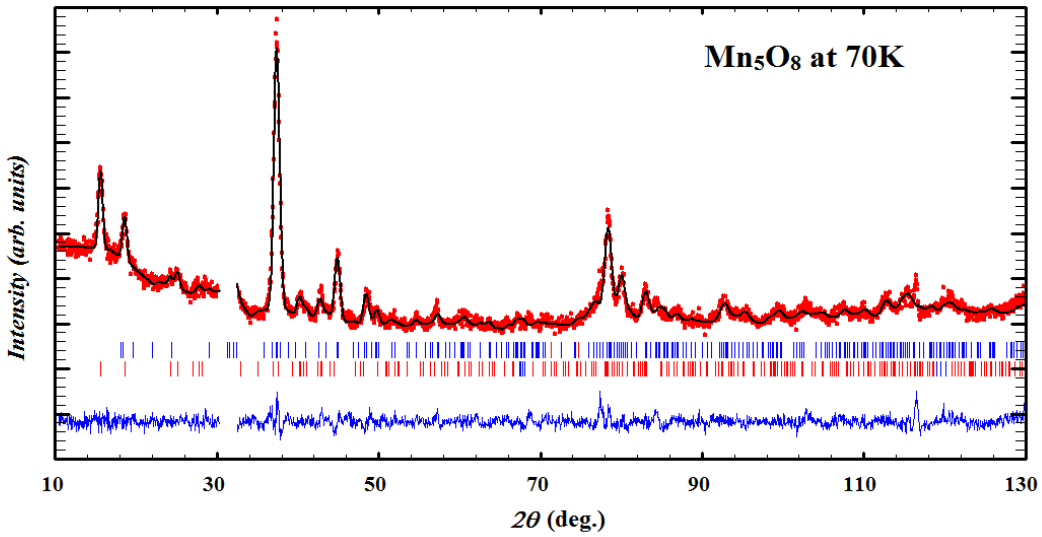

Figure 1: Experimental, calculated, and difference NPD patters of Mn_5O_8 at 70 K. Upper and lower bars denote Bragg positions of nuclei and magnetic reflections respectively. The region 30.2^o to 32.3^o is excluded owing to background from the detector system.

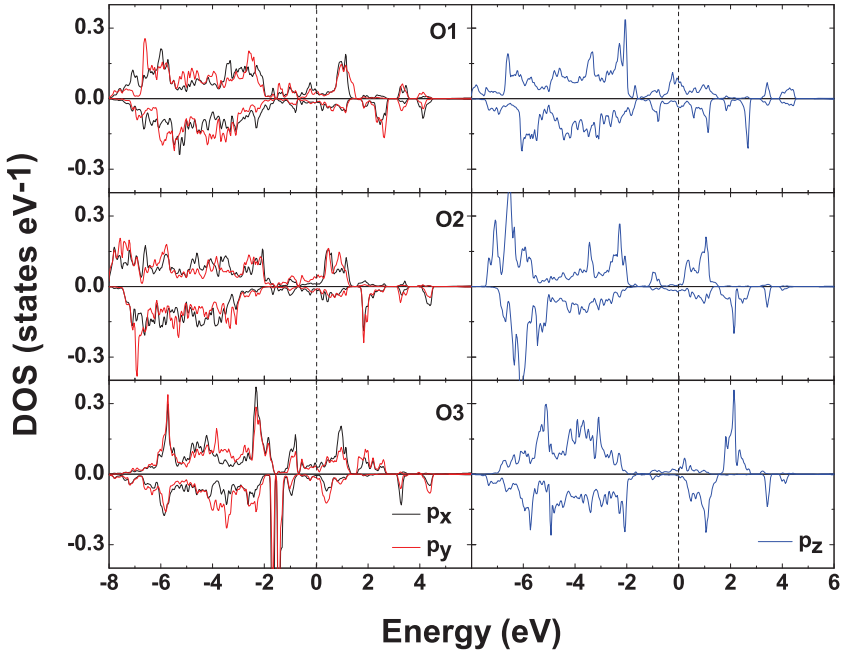

Figure 2: Orbital decomposed DOS for oxygen p states of Mn_5O_8 in the ground state M4 configuration.

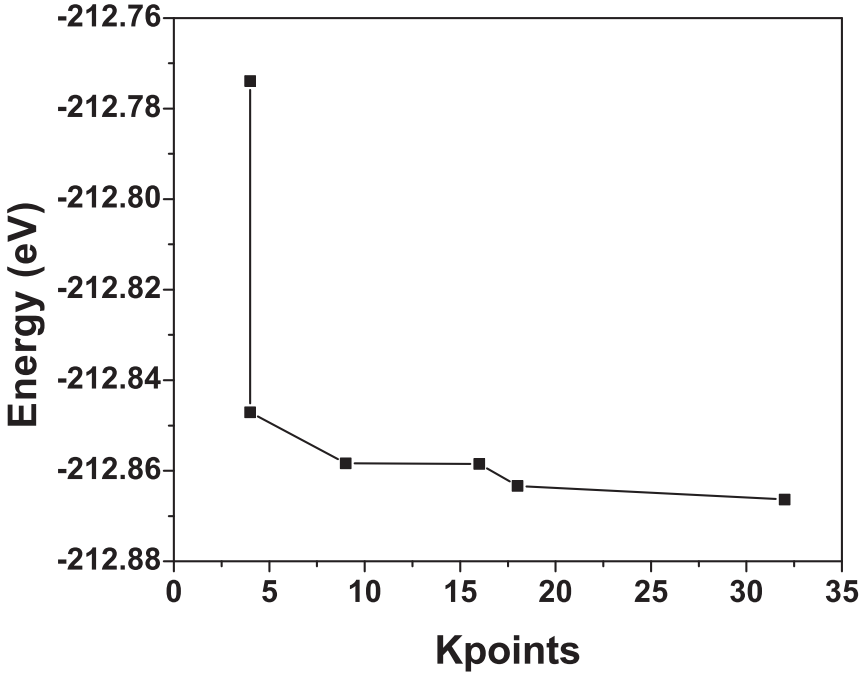

Figure 3: Total energy curve as a function of K-point for Mn_5O_8