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

Theoretical Investigation of Quantum Capacitance of Co-doped α-MnO_2 for Supercapacitor Application using Density Functional Theory

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Supporting Information

1. Computational Details for Dispersion Correction

To incorporate the effect of dispersion interactions in the formation energy, the semi-empirical method proposed by Grimme (DFT-D2) was used.

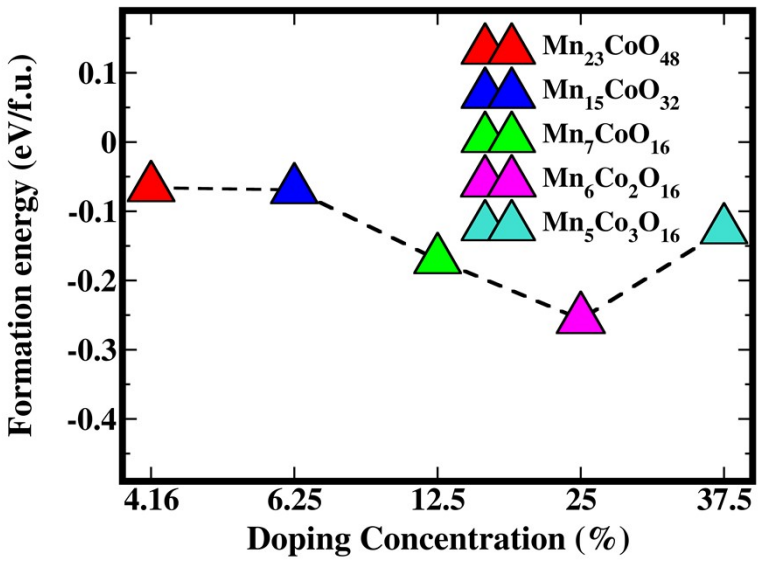

Fig. S1: Variation of formation energy using dispersion correction with increasing doping concentration.