Supplementary Information

Comment on "Crystal growth and aggregation in suspensions of δ-MnO_2 nanoparticles: implications for surface reactivity" by F. F. Marafatto, B. Lanson and J. Peña, *Environ. Sci.: Nano*, 2018, 5, 497

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Table S1. Atomic coordinates and site occupancies used to calculate the XRD profiles and to fit the δ-MnO_2 sample pattern from Fig. 3A. Same conventions as in Table 3 from Ref. [18].

	Coordinates			
Atom	**x**	**y**	**z**	**Occupancy**
^{E}Mn (Mn1)	0	0	0	0.90
O_{Mn1}	0.333	0	0.14	2.0
^{TC}Mn (Mn2)	0	0	0.29	0.05
O_{Mn2}	-0.333	0	0.45	0.15
Interlayer Na	-0.540	0	0.5	0.083
	-0.230	0.310	0.5	0.083
	-0.230	-0.310	0.5	0.083
Interlayer Water	0.120	0	0.5	0.083
	-0.06	0.18	0.5	0.083
	-0.06	-0.18	0.5	0.083

a = 4.919 Å; b = 2.84 Å; c = 7.20 Å, α = β = γ = 90°. Debye–Waller factors B (Å2) were fixed to 0.5 for Mn1, 1.0 for O1 and Mn2, and 2.0 for all other atoms

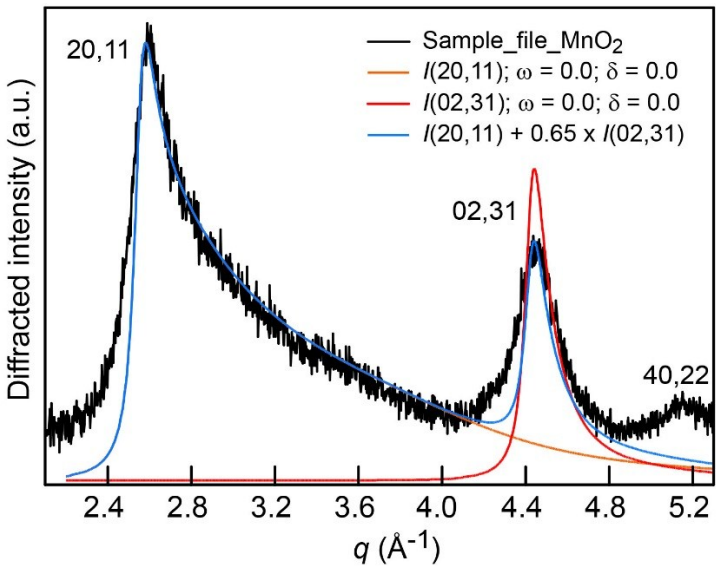

Fig. S1. Reconstruction of the δ-MnO_2 pattern shown in Fig. 3A by adding the 20,11 and 02,31 line profiles calculated separately and without considering microstrain resulting from particle bending. In this way, the strain effect in the pattern apparently can be reproduced by (1) adjusting the calculated *I*(20,11) / *I*(02,31) ratio to *I*(20,11) / [0.65 x *I*(02,31)], and (2) increasing the width of the 02,31 line, i.e., changing the CSD dimension (not shown in the Figure).