Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

An Experimental and Computational Study to Understand the Lithium Storage Mechanism in Molybdenum Disulphide

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Table T1: Best fit parameters for EXAFS fitting

		MoS_2			**MoO_3**				
		Mo-S	**Mo-Mo**						
MoS_2	Theoretical R; CN	2.43; 6	3.17; 6						
	R	2.39	3.13						
	Amp	0.93	0.98						
	N	6	6						
	CN	5.6	5.9						
	enot	2.88	-3.87						
	Ss2	0.0044	0.0083						
	R-factor	0.08							
		Mo-S	**Mo-O**	**Mo-S**	**Mo-O**	**Mo-O**	**Mo-O**	**Mo-O (combined)**	
After 1st Discharge	Theoretical R; CN	2.43; 6	3.17; 6	3.99; 6	1.57; 1	1.75; 1	1.93; 2	2.37; 2	
	R	2.36	3.47	3.78	1.55	1.87	2.26	2.39	
	Amp	0.22	0.39	0.64	0.73	1.36	1.79	0.16	
	N	6	6	6	1	1	2	2	
	CN	1.3	2.3	3.8	0.7	1.4	1.8	0.4	
	enot	11.2	21.6	11.2	21.2	21.2	21.2	21.2	
	Ss2	0.0019	0.0027	0.0084	0.009	0.0013	0.0031	0.0036	
	R-factor	0.05							
		Mo-S	**Mo-O**		**Mo-O**	**Mo-O**	**Mo-O**	**Mo-O**	**Mo-O**
After 10th Discharge-trial 2	Theoretical R; CN				1.57; 1	1.75; 1	1.93; 2	2.37; 1	2.40; 1
	R				1.61	1.72	1.73	2.14	2.51
	Amp				0.7	0.82	0.71	1.31	2.08
	N				1	1	2	1	1
	CN				0.7	0.8	1.4	1.3	2.1
	enot				2.7	2.7	2.7	2.7	2.7
	Ss2				0.01	0.0015	0.0004	0.002	0.0023
	R-factor	0.066							