

ESI file for

Probing room-temperature reactivity of H₂S, SO₂, and NO on Li₂MnO₃ crystal surface by experimental and first-principles studies

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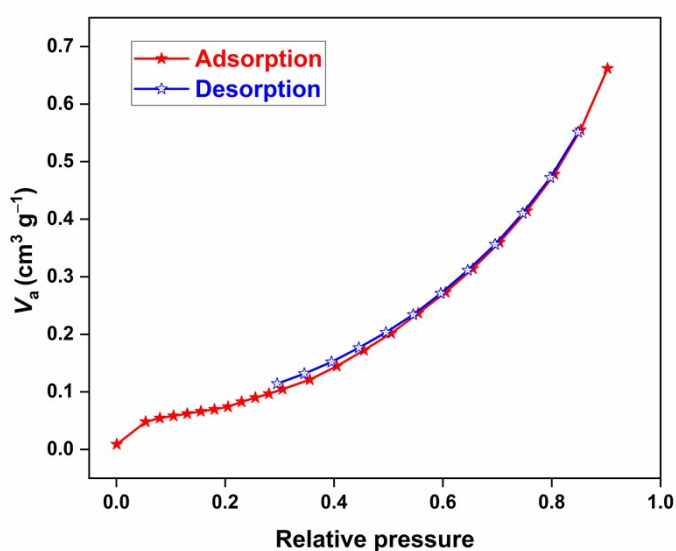


Figure S1. N₂ adsorption-desorption isotherm of Li₂MnO₃.

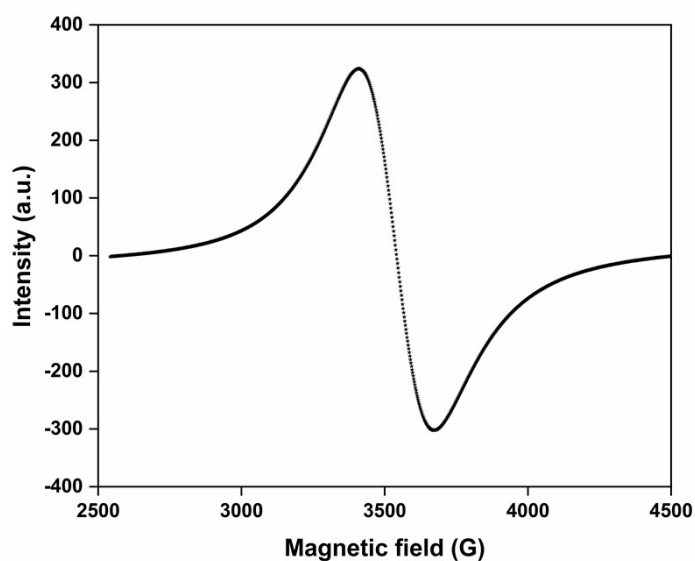


Figure S2. EPR spectrum of Li₂MnO₃.

Table S1. The peak-fitting results of O 1s high-resolution signal of fresh and gas-exposed samples.

Samples	Assignment	E_B (eV)	FWHM (eV)	At. %
Li₂MnO₃	O–Li, O–Mn	530.0	1.2	70.9
	OH surf	531.6	1.8	22.0
	water	533.0	1.9	7.1
Li₂MnO₃_SO₂	O–Li, O–Mn	530.0	1.2	67.6
	OH surf	531.7	1.7	20.4
	water	532.8	1.8	12.0
Li₂MnO₃_H₂S	O–Li, O–Mn	530.1	1.4	45.5
	OH surf	531.7	1.7	25.3
	water	532.8	1.9	29.2
Li₂MnO₃_NO	O–Li, O–Mn	530.0	1.2	58.1
	OH surf	531.6	1.8	20.5
	water	533.1	1.9	21.4

Table S2. The peak-fitting results of Mn 2p_{3/2} high-resolution signal of fresh and gas-exposed samples.

Samples	Assignment	E_B (eV)	FWHM (eV)	At. %
Li₂MnO₃	Mn ²⁺	640.5	1.2	10.9
	Mn ³⁺	641.8	1.2	37.2
	Mn ⁴⁺	642.9	1.8	51.9
	Satellite	644.8	2.0	-
Li₂MnO₃_SO₂	Mn ²⁺	640.8	1.2	11.8
	Mn ³⁺	642.1	1.2	43.4
	Mn ⁴⁺	643.2	1.6	44.8
	Satellite	644.3	2.5	-
Li₂MnO₃_H₂S	Mn ²⁺	640.9	1.2	11.9
	Mn ³⁺	642.2	1.5	41.8
	Mn ⁴⁺	643.4	1.9	46.3
	Satellite	644.3	2.6	-
Li₂MnO₃_NO	Mn ²⁺	640.8	1.2	10.7
	Mn ³⁺	642.0	1.2	39.9
	Mn ⁴⁺	643.1	1.7	49.4
	Satellite	644.8	2.1	-

Table S3. The peak-fitting results of S 2p_{3/2} high-resolution signal of fresh and gas-exposed samples.

Samples	Assignment	E_B (eV)	FWHM (eV)	At. %
Li₂MnO₃_SO₂	Sulphate	168.8	2.0	100
Li₂MnO₃_H₂S	Sulphide	162.2	1.1	3.4
	Sulphur	164.2	1.7	13.4
	Sulphate	169.3	2.1	83.3

Table S4. The peak-fitting results of N 1s high-resolution signal of fresh and gas-exposed samples.

Sample	Assignment	E_B (eV)	FWHM (eV)	At. %
Li₂MnO₃_NO	NO(1)	399.7	1.7	64.0
	NO(2)	401.7	1.7	36.0