Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supporting Information

Consistent interpretation of isotope and chemical oxygen exchange relaxation kinetics in SrFe_{0.85}Mo_{0.15}O_{3-δ} ferrite

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Table S1. Experiment parameters

	Flow	Rector	T, °C	<i>p</i> O ₂ , atm
QEOR	50 ml/min	Tubular quartz, 4 mm inner diameter	600-900	10 ⁻⁵ -0.2
OPPR	10-45 ml/min	Tubular quartz, 4 mm inner diameter	650-850	10 ⁻³ -10 ⁻¹ atm
IE	static	cylindrical reactor, 15 cm ³	600-640	





Fig. S2 – SEM images of the cylinder used in OPPR a) surface, b) cross-section





Table S2. Experimental and modeling error details

Step	J	p ⁰ _{des}	p ⁰ _{ads}	χ^2 normal	R _{factor}	R ₀₀	±Er(R ₀₀)	D _{chem}	±Er(D)		
850											
7/5	25	0.06892	0.04842	3.29E-5	0.99998	1.56E-06	1.67E-08	2.80E-05	1.97E-07		
3/2	25	0.02835	0.01848	1.65E-5	0.99999	1.40E-06	3.83E-09	2.15E-05	8.02E-08		
1.5/1	25	0.01354	0.0087	4.05E-5	0.99998	1.42E-06	1.89E-09	1.87E-05	2.65E-08		
0.7/0.5	35	0.00664	0.00467	5.3E-5	0.99997	1.37E-06	5.73E-09	1.65E-05	1.72E-07		
0.3/0.2	45	0.00279	0.00182	5.99E-5	0.99997	1.25E-06	4.58E-09	1.29E-05	2.59E-07		
800											
7/5	20	0.06737	0.0477	2.05E-5	0.99999	1.00E-06	8.25E-09	1.92E-05	1.01E-07		
3/2	25	0.02878	0.01902	3.17E-5	0.99998	1.06E-06	5.64E-09	1.52E-05	9.66E-08		
1.5/1	25	0.0141	0.00933	1.94E-5	0.99999	1.02E-06	2.85E-09	1.34E-05	5.23E-08		
0.7/0.5	35	0.00661	0.00468	8.08E-5	0.99996	9.53E-07	4.22E-09	1.12E-05	1.09E-07		
0.3/0.2	45	0.00279	0.00184	9.23E-5	0.99995	9.22E-07	3.00E-09	8.15E-06	8.48E-08		
750											
7/5	15	0.06451	0.0458	1.05E-5	0.99999	6.30E-07	2.10E-09	1.07E-05	5.47E-08		
3/2	25	0.02886	0.01906	1.37E-5	0.99999	6.13E-07	2.05E-09	9.11E-06	4.77E-08		
1.5/1	25	0.01411	0.00933	2.24E-5	0.99999	6.01E-07	1.59E-09	7.71E-06	3.79E-08		
0.7/0.5	35	0.00665	0.00466	4.49E-5	0.99998	6.07E-07	1.71E-09	7.13E-06	5.34E-08		
0.3/0.2	40	0.00281	0.00181	1.23E-4	0.99994	5.68E-07	2.19E-09	5.12E-06	8.35E-08		
700											
7/5	10	0.06032	0.04272	3.51E-5	0.99998	3.65E-07	2.25E-09	7.05E-06	5.17E-08		
3/2	20	0.02819	0.01871	1.37E-5	0.99999	3.26E-07	1.13E-09	6.12E-06	4.39E-08		
1.5/1	20	0.01385	0.0092	4.07E-5	0.99998	3.09E-07	1.09E-09	4.70E-06	3.59E-08		
0.7/0.5	25	0.00652	0.00462	2.82E-4	0.99986	2.89E-07	1.94E-09	3.92E-06	8.04E-08		
0.3/0.2	25	0.00279	0.00187	2.59E-4	0.99987	3.04E-07	1.41E-09	3.29E-06	5.30E-08		
650											
7/5	10	0.06013	0.04281	5.22E-5	0.99997	1.33E-07	9.46E-10	3.60E-06	1.57E-08		
3/2	10	0.02505	0.0167	6.01E-5	0.99997	1.31E-07	7.10E-10	3.05E-06	3.02E-08		
1.5/1	15	0.01317	0.00877	1.08E-4	0.99995	1.26E-07	8.24E-10	2.51E-06	1.08E-07		
0.7/0.5	15	0.00595	0.00435	3.07E-4	0.99985	1.25E-07	1.07E-09	2.22E-06	9.29E-08		
0.3/0.2	15	0.0025	0.0018	0.00172	0.99914	1.25E-07	1.99E-09	1.84E-06	2.13E-07		

*J – total gas flow rate, ml/min; p_{des}^0 , p_{ads}^0 – initial oxygen partial pressure at desorption and adsorption stage, atm; χ^2_{normal} – normalized square of relative data description error; R_{factor} - measure of the disagreement between the modeled and observed amplitudes, $R_{00} = R_0/p^n$ - pre-exponential factor of exchange rate constant; D_{chem} - chemical diffusion coefficient, cm² s⁻¹



