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

Electronic Supplementary Information

A Comprehensive diffusion-induced stress coupled multiscale modeling and analysis in hard-carbon electrode of Li-ion batteries

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Table S1. The current densities (mA/cm^2) applied to particles of various radius at different C-rates.

S. No.	Radius of the particle (nm)	Applied current density (mA/cm^2)			
		@ 1 C rate	@ 2 C rate	@ 5 C rate	@ 10 C rate
1	100	0.004167	0.008333	0.020833	0.041667
2	200	0.008333	0.016667	0.041667	0.083333
3	300	0.012500	0.025000	0.062500	0.125000
4	400	0.016667	0.033333	0.083333	0.166667
5	500	0.020833	0.041667	0.104167	0.208333
6	600	0.025000	0.050000	0.125000	0.250000
7	700	0.029167	0.058333	0.145833	0.291667
8	800	0.033333	0.066667	0.166667	0.333333
9	900	0.037500	0.075000	0.187500	0.375000
10	1000	0.041667	0.083333	0.208333	0.416667

Table S2. Diffusivity (D) of Li^+ in Li_xC at room temperature (300 K) and Elastic modulus (E) of Li_xC calculated using the MD simulation, with ReaxFF potential.

Phase/SOC (%)	**Diffusivity (D in cm^2/s)**	**Elastic modulus (E in GPa)**
$Li_{0.0224}C$ / SOC (10%)	1.96×10^{-11}	53.99
$LI_{0.0448}C$ / SOC (20%)	5.84×10^{-11}	52.91
$LI_{0.0672}C$ / SOC (30%)	2.08×10^{-11}	49.41
$LI_{0.0896}C$ / SOC (40%)	5.52×10^{-11}	41.58
$LI_{0.112}C$ / SOC (50%)	6.76×10^{-11}	31.73
$Li_{0.1344}C$ / SOC (60%)	2.15×10^{-10}	35.02
$Li_{0.1568}C$ / SOC (70%)	3.01×10^{-10}	30.49
$Li_{0.1792}C$ / SOC (80%)	4.82×10^{-10}	29.47
$Li_{0.2016}C$ / SOC (90%)	1.99×10^{-11}	20.22

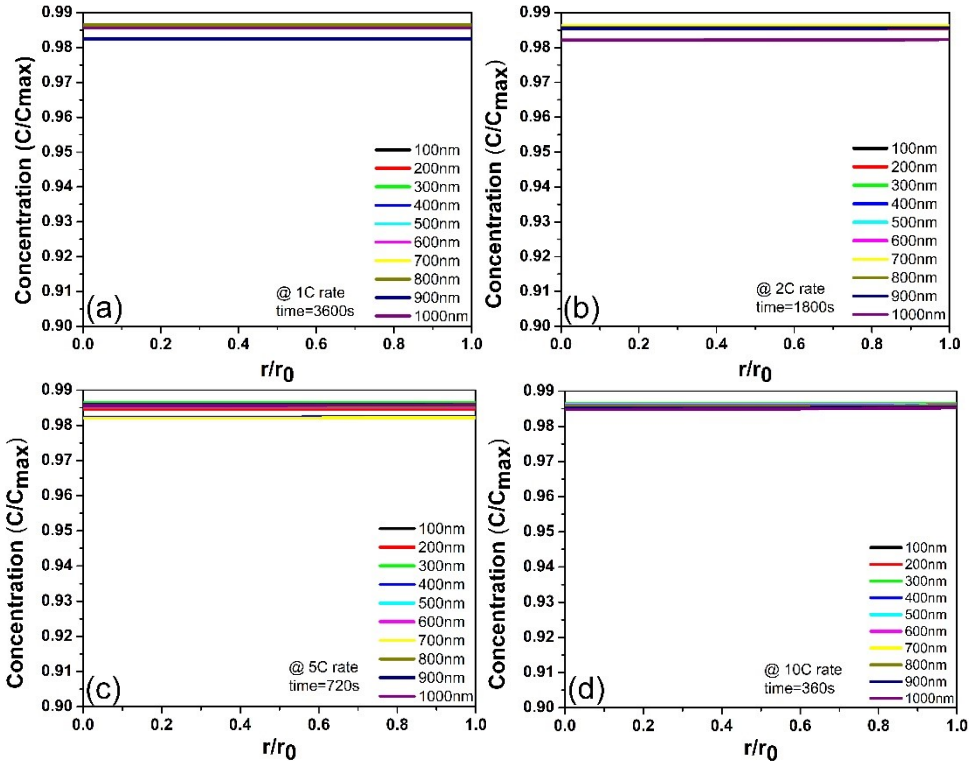

Fig. S1 Evolution of the particle size-dependent dimensionless concentration field for the two-way coupled approach over the dimensionless radius at (a)1C, (b) 2C, (c) 5C, and (d)10C-rates. All the profiles were shown for the corresponding last times steps (SOC 100) for different particle size (100-1000 nm).

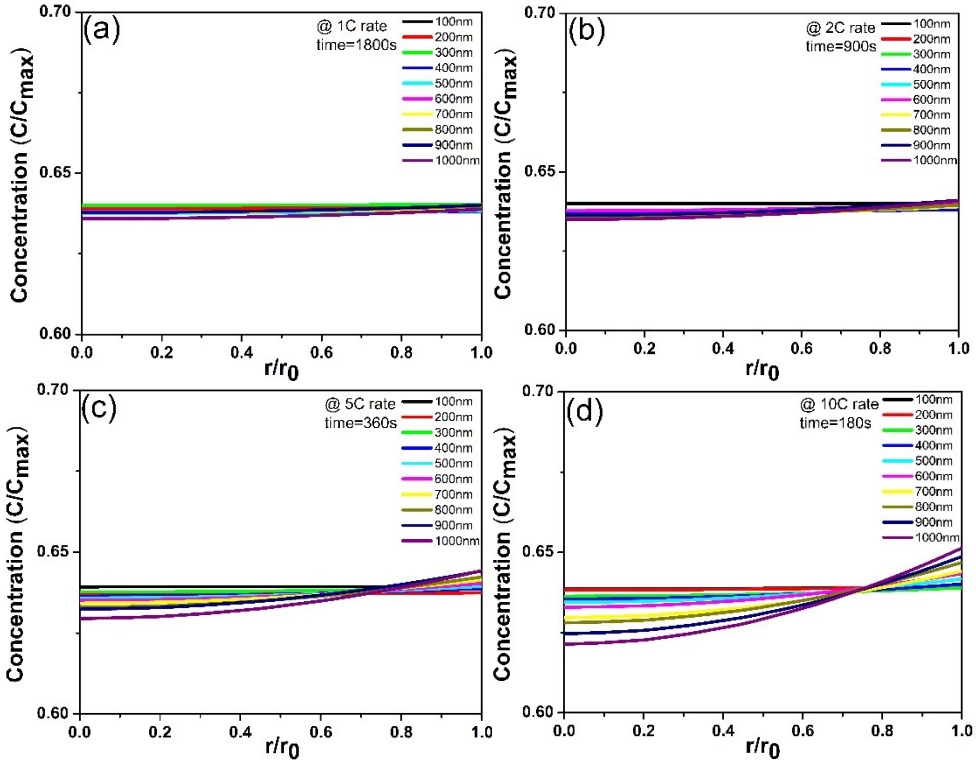

Fig. S2 Evolution of the particle size-dependent dimensionless concentration field for the two-way coupled approach over the dimensionless radius at (a)1C, (b) 2C, (c) 5C, and (d)10 C-rates. All the profiles were shown for the corresponding half of the lithiation time. (e) values of the Li+ concentration at half of the particle radius for all the particles with respect to C-rates and (f) schematic of the spherical particle showing the location of r/r0 where the values of concentration are obtained.

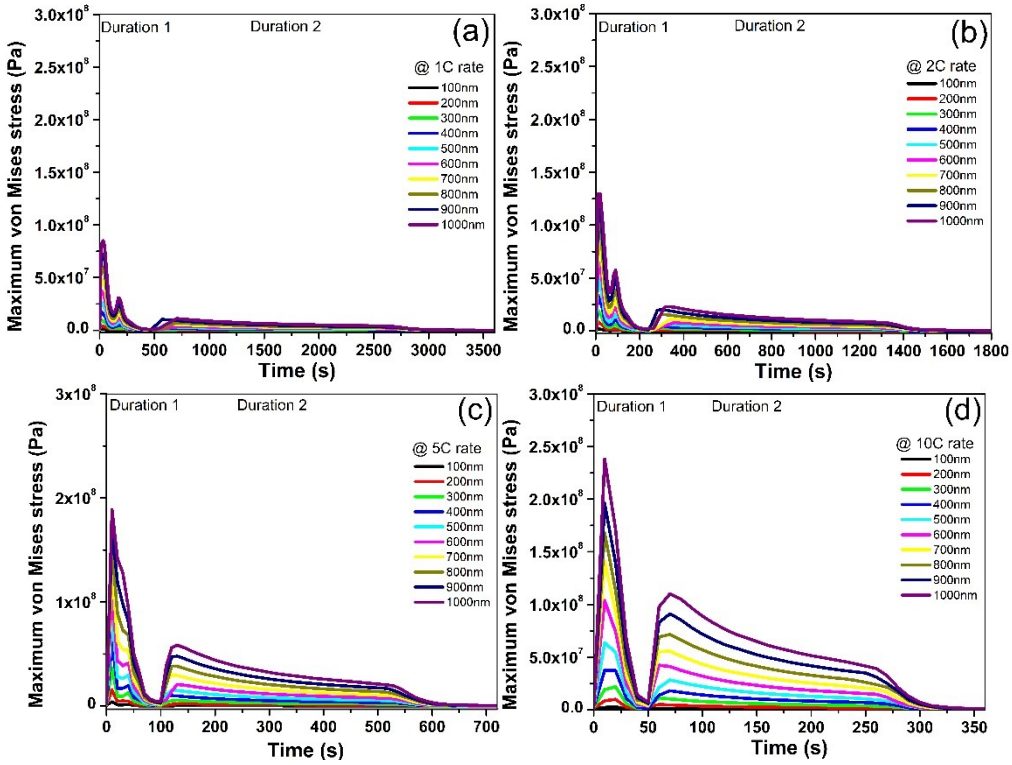

Fig. S3 Maximum von Mises stress over time, for different spherical particles of radius 100-1000 nm, for the two-way coupled approach over different lithiation rates (C-rates), (a) 1C, (b) 2C, (c) 5C, and (d) 10C, peak values of maximum von Mises stresses with respect to C-rate for various particle sizes at (e) duration 1 (up to SOC 15), and (f) duration 2 (SOC range 15-100). (One-way coupled)