Electronic signatures of anharmonic dynamics and charge fluctuations in Lithiated graphite

Sasawat Jamnuch[1] and Tod A Pascal[1,2,3*]

[1]Nano and Chemical Engineering, University of California San Diego, La Jolla, CA, USA 92023

[2]Material Science and Engineering, University of California San Diego, La Jolla, CA, USA, 92023

[3]Sustainable Energy and Power Center, University of California San Diego, La Jolla, CA, USA, 92023

Correspondence: tpascal@ucsd.edu

Supplementary Materials

Supplementary Tables

Table S1: Distribution analysis of in-plane and out-of-plane Li atom displacement with staging

System	Mean		Standard deviation		Skewness		Kurtosis	
	In-plane	*Out of plane*	*In-plane*	*Out of plane*	*In-plane*	*Out of plane*	*In-plane*	*Out of plane*
Stage I	0.0004	0.0001	0.1185	0.0488	-0.0090	0.0045	2.9220	2.9705
Stage II	-0.0008	-0.0003	0.1821	0.0895	-0.0115	-0.1352	2.7856	5.2158
Stage III	0.0024	-0.0012	0.1316	0.0792	0.0686	0.0089	3.2412	3.6322

Table S2: Distribution analysis of C atom charge fluctuations with staging

System	Mean	Standard deviation	Skewness	Kurtosis
Stage I	-0.14428	0.03617	0.11853	2.75536
Stage II	-0.07210	0.03991	0.21840	2.80112
Stage III	-0.02860	0.08294	-0.22227	3.01854
Graphite	-0.00000	0.09978	-0.08057	2.67974

Supplementary Figures

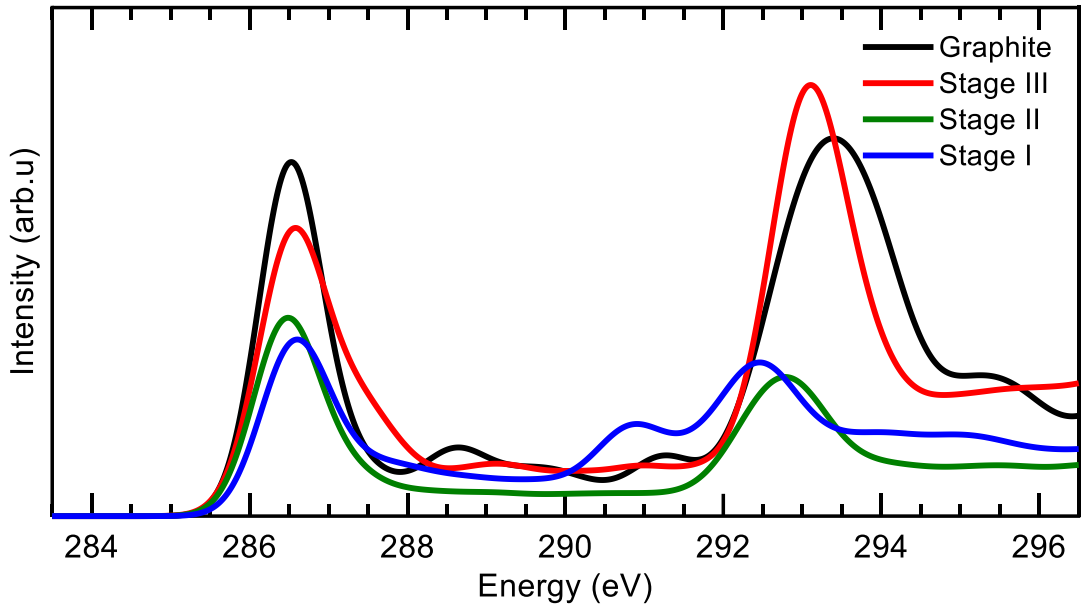

Figure S1: Simulated Carbon K-edge XAS of graphite and LiGCs based on the pristine crystal structure

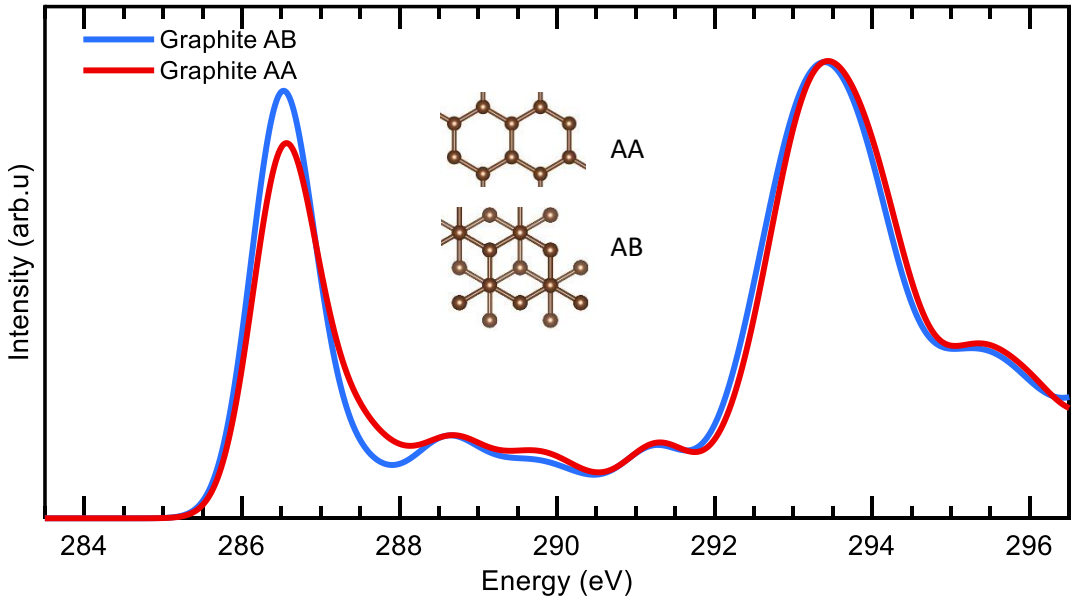

Figure S2: Simulated Carbon K-edge XAS of graphite between the AA and AB stacked structures.

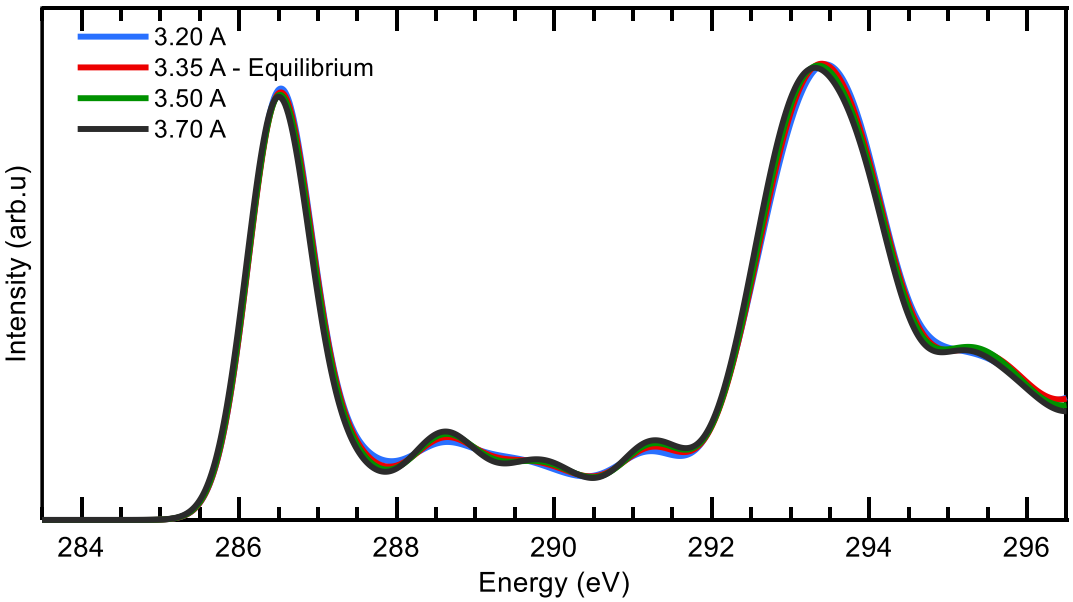

Figure S3: Simulated Carbon K-edge XAS of graphite as a function of sheet-sheet interlayer distance.

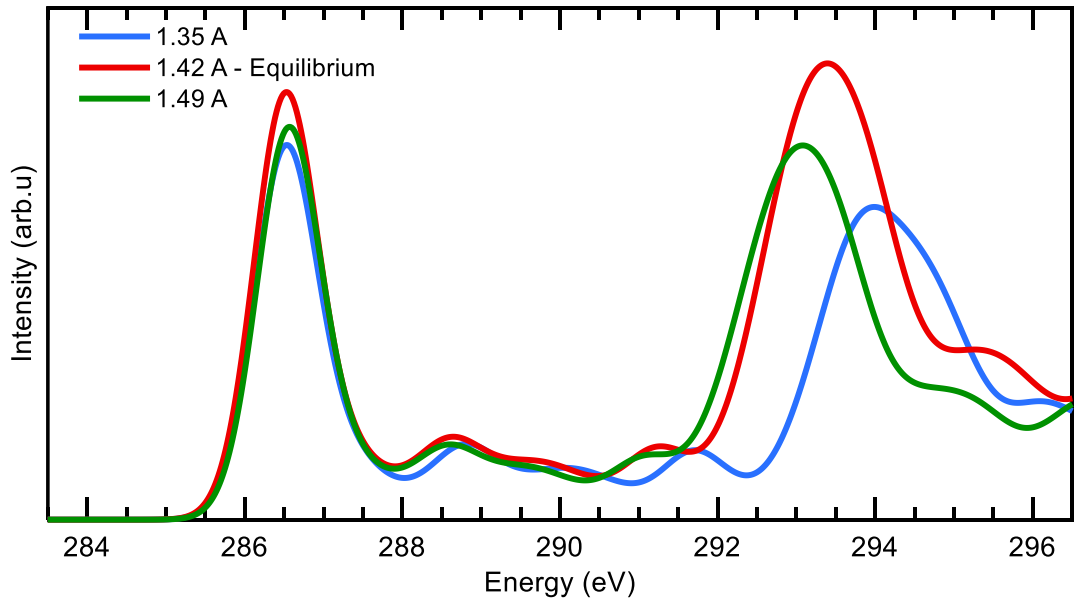

Figure S4: Simulated Carbon K-edge XAS of AB stacked graphite as a function of in-place lattice constant

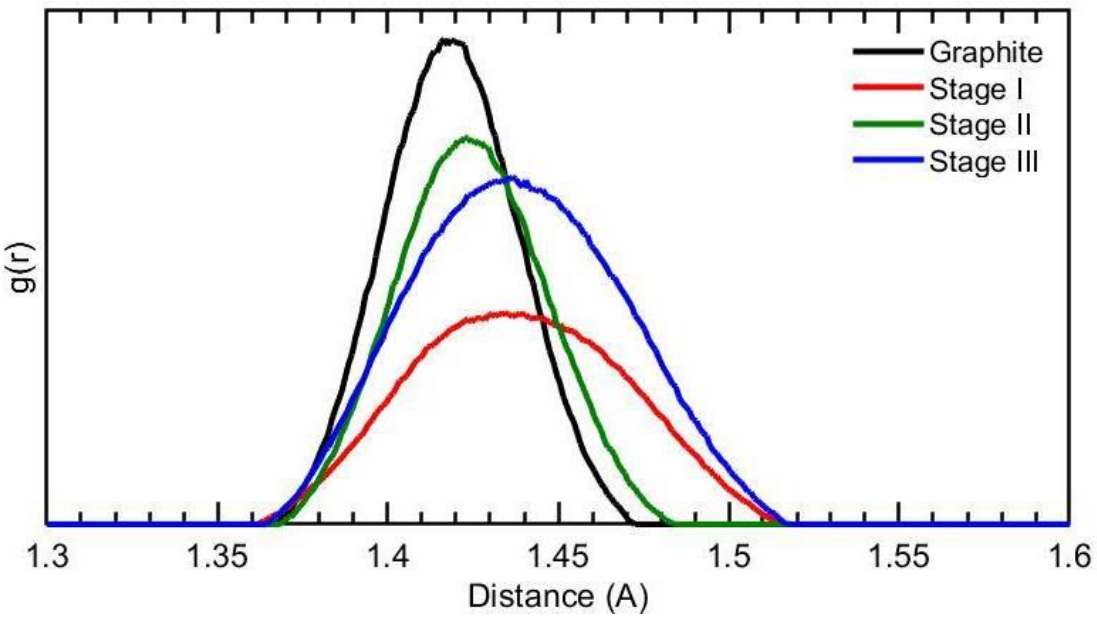

Figure S5: Carbon – Carbon radial distribution function in graphite and Li-GICs

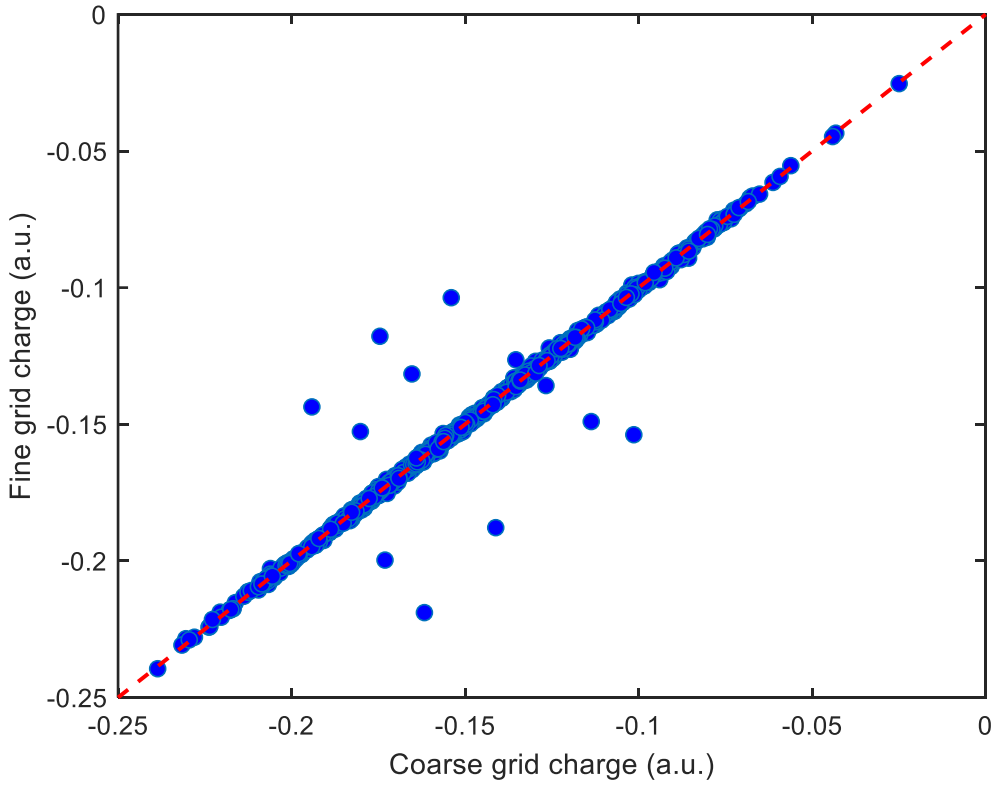

Figure S6: Bader charge analysis comparison between coarse and fine k-point grids