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Supporting information

Structure-property relationships in organic battery anode materials: exploring redox reactions in crystalline Na- and Li-benzene diacrylate using combined crystallography and density functional theory calculations

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Table S1 *Space group of all crystal structures as theoretically predicted.*

	Na_2BDA	**Li_2BDA**
Pristine	$P2_1/c$	$P2_1/c$
1st ion insertion	P1	$P\bar{1}$
2nd ion insertion	$P2_1/c$	$P\bar{1}$

Table S2 *Lattice parameters of all crystal structures as theoretically predicted.*

	Na_2BDA	**Na_3BDA**	**Na_4BDA**	**Li_2BDA**	**Li_3BDA**	**Li_4BDA**
a (Å)	13.77	15.02	14.03	11.11	13.03	13.33
b (Å)	5.34	5.39	5.11	5.36	5.13	5.28
c (Å)	6.89	6.72	8.09	8.28	7.57	7.59
α (deg)	90.01	90.01	90.05	89.97	86.84	86.40
β (deg)	97.31	78.05	76.64	90.05	100.15	107.03
γ (deg)	89.95	96.09	90.05	87.15	86.80	101.05

Table S3 *Comparison of experimental data between the PXRD-Na_2BDA and SCXRD-Li_2BDA.*

Parameter	**Na_2BDA**	**Li_2BDA**
Molar mass (g/mol)	262.02	230.07
Temp of measurement (K)	293	293
Space group	$P\,2_1/c$	$P\,2_1/c$
a axis (Å)	14.53	13.75
Cell volume (Å^3)	526.35	1170.99
Z	2	4
Calc. density (g/cm^3)	1.65429	1.39586
Crystal colour	white	white

The predicted lithiated phases for the Li_2BDA compound are presented on the Figure S1.

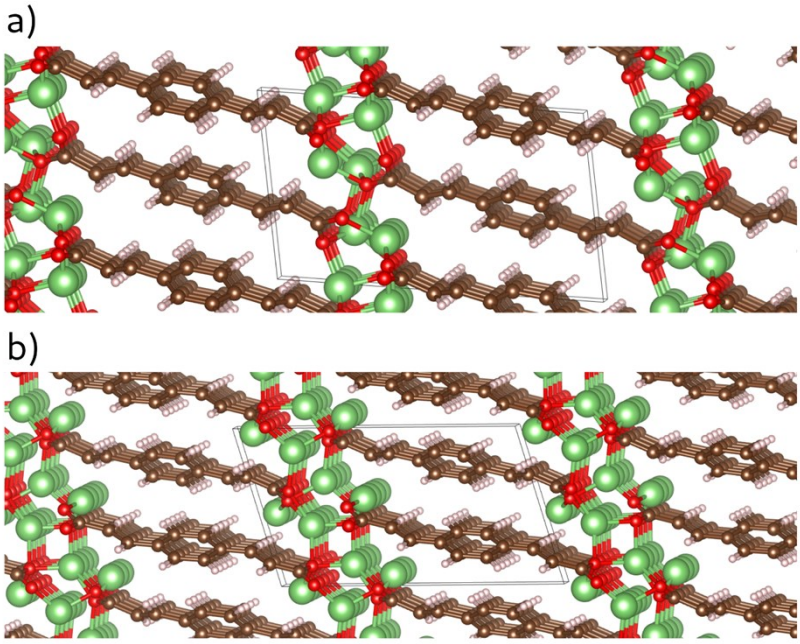

Figure S1 *The predicted crystal structure for the lithiated phases a) Li_3BDA and b) Li_4BDA.*

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3D electron diffraction

The sample was crushed in an agate mortar, dispersed in absolute ethanol. A droplet of the suspension was transferred onto a copper grid covered by a holey carbon film. The 3D electron diffraction data were collected using a JEOL JEM-2100 transmission electron microscope (TEM) operated at an accelerating voltage of 200 kV. The data were collected by continuously tilting the goniometer with a tilt speed of 0.28 °/s. During tilting the crystal was tracked by sequential defocusing of the intermediate lens using the software Instamatic.[1] The data were collected using the hybrid detection camera Timepix (ASI). Intensity extraction was performed using X-ray Detector Software (XDS)[2]. The structure was solved using the software SHELXT[3], the positions of all non-hydrogen atoms were directly obtained with reasonable geometries. A least-squares refinement was performed in SHELXL[4] using atomic scattering factors for electrons extracted from SIR2014[5]. The refinement converged with an R1 of 35% without the use of restraints. Details regarding the data and structure refinement can be found in Table S4.

Table S4. *Details of the electron diffraction data and refinement.*

Crystal system	Monoclinic
Space group	$P2_1/c$ (No. 14)
a, Å	14.49
b, Å	5.50
c, Å	7.21
α, °	90
β, °	101.1
γ, °	90
Volume, Å^3	563.9
λ, Å	0.0251
Exposure time per frame (s)	0.6
Tilt range, °	-58.3 – +62.3
Resolution, Å	0.9
Completeness, %	77.2
R_{int}	0.1142
R1	0.3535
No. of symmetry independent reflections	617
Restraints	0

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