Supporting Information for

Planar NiC_3 as a Reversible Anode Material with High Storage Capacity for Lithium-Ion and Sodium-Ion Batteries

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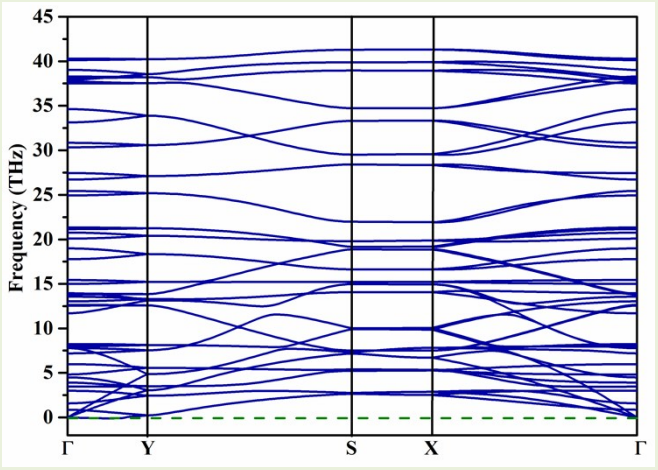

Figure S1. Phonon dispersion of NiC_3 monolayer computed using the PBE functional.

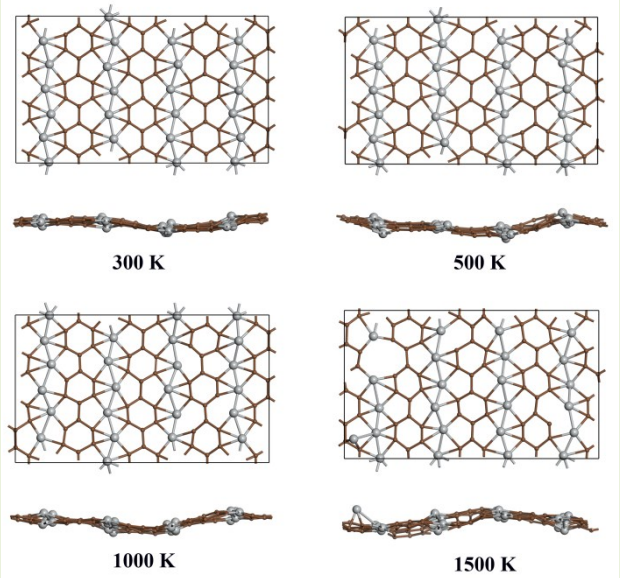

Figure S2. Snapshots of NiC_3 monolayers equilibrium structures at 300 K, 500 K, 1000 K, 1500 K at the end of 10 ps AIMD simulations.

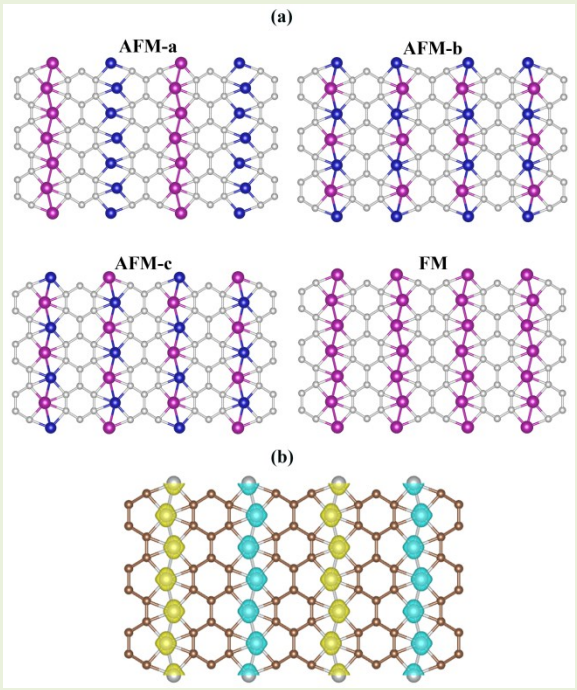

Figure S3. (a) Three different antiferromagnetic spin density distributions (AFM-a, AFM-b and AFM-c) of NiC_3 monolayer. Pink and blue denote two opposite spin orientations; (b) Spin-polarized density of the ground state NiC_3 monolayer in the 3D isosurface version with a value of 0.005 au. Yellow and light blue denote two opposite spin orientations.

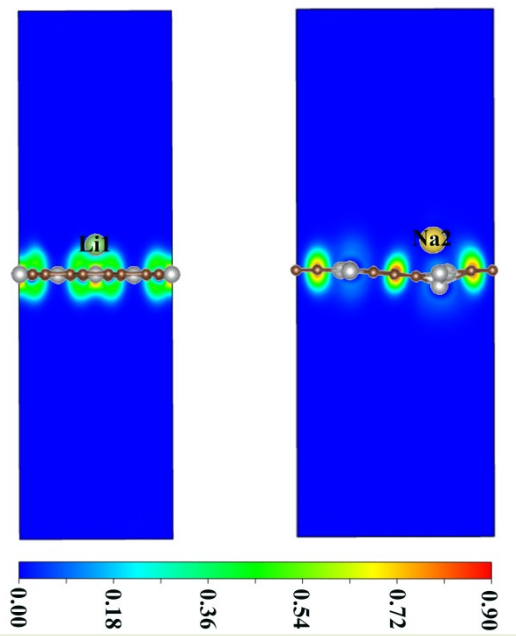

Figure S4. ELF map of NiC_3 monolayer adsorbing one Li-ion and one Na-ion.

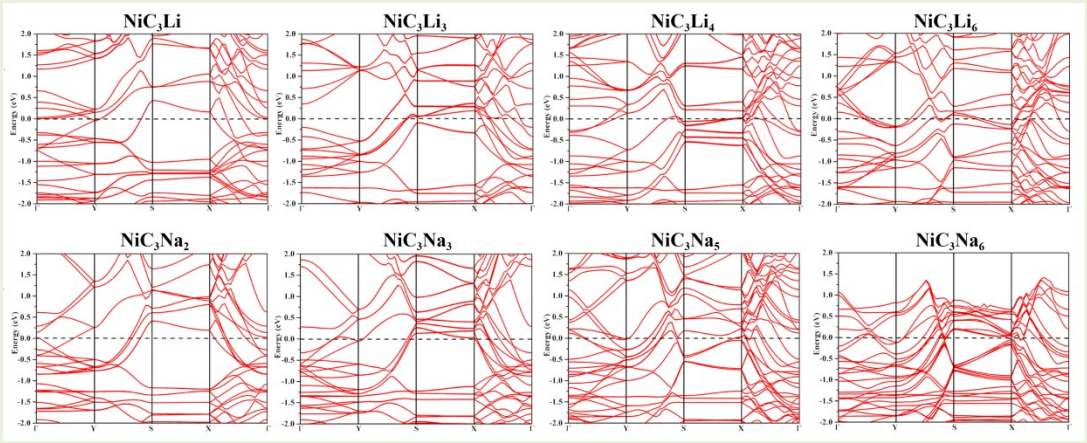

Figure S5. Electronic band structure of NiC_3Li, NiC_3Li_3, NiC_3Li_4, NiC_3Li_6, NiC_3Na_2, NiC_3Na_3, NiC_3Na_5 and NiC_3Na_6 monolayers calculated at the PBE level, respectively. The Fermi levels are all set to zero.

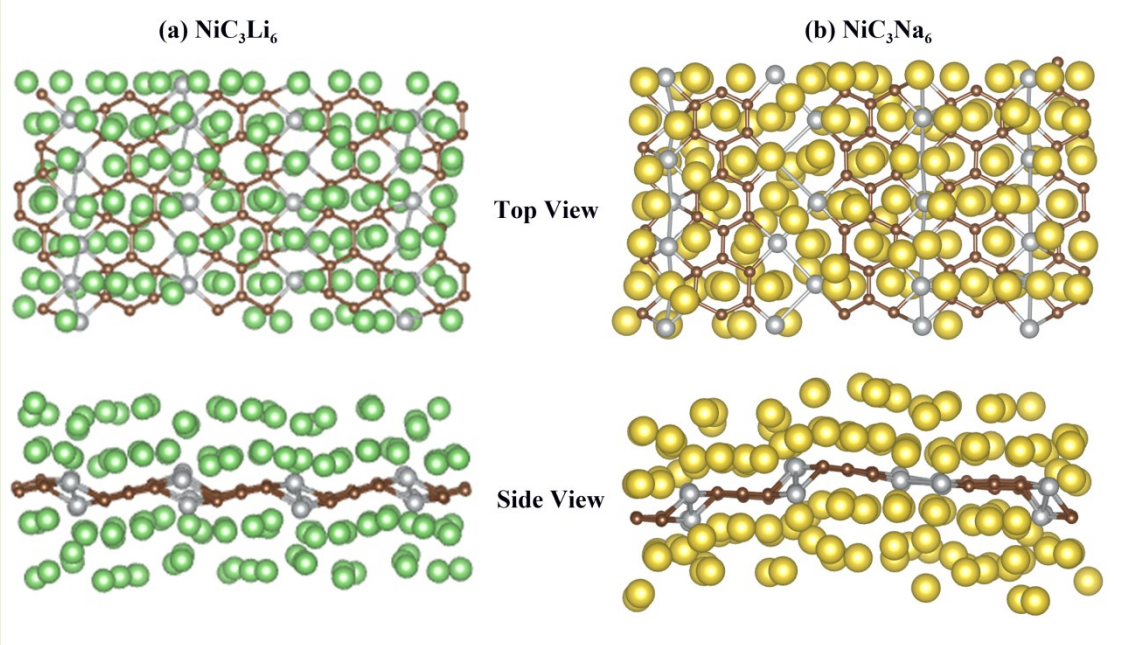

Figure S6. Snapshots of (a) NiC_3Li_6 and (b) NiC_3Na_6 equilibrium structures at 300 K at the end of 10 ps AIMD simulations.

Table S1. Structural information of the optimized NiC_3 monolayer.

Phase	Space Group	Lattice Parameters (Å, º)	Coordinates
NiC_3	CMMM	a =11.22181	Ni(0.227301627,0.500000000,0.500000000)
		b =4.35599	Ni(0.772695899,0.500000000,0.500000000)
		c=30.00000	Ni(0.727304041,0.000000000,0.500000000)
		α=β=γ=90.00000	Ni(0.272698462,0.000000000,0.500000000)
			C(0.000000000,0.333009481,0.500000000)
			C(0.000000000,0.666990519,0.500000000)
			C(0.499999821,0.833009481,0.500000000)
			C(0.499999821,0.166990504,0.500000000)
			C(0.891456366,0.838617027,0.500000000)

			C(0.108544089,0.161381647,0.500000000)
			C(0.108544089,0.838618338,0.500000000)
			C(0.891456366,0.161382943,0.500000000)
			C(0.391455889,0.338618428,0.500000000)
			C(0.608543754,0.661383033,0.500000000)
			C(0.608543754,0.338616997,0.500000000)
			C(0.391455889,0.661381602,0.500000000)

Table S2. Structural information of the optimized $Ni_8C_{24}Li1$.

Phase	Space Group	Lattice Parameters (Å, º)	Coordinates
$Ni_8C_{24}Li1$	PMM2	a =11.26541	Ni(0.226504043,0.249999568,0.500999212)
		b =8.70284	Ni(0.773496091,0.250000387,0.501004577)
		c=30.00000	Ni(0.728317201,0.999846935,0.499485135)
		α=β=γ=90.00000	Ni(0.271684021,0.999848425,0.499486744)
			Ni(0.227969095,0.750000358,0.500962019)
			Ni(0.772032559,0.749999702,0.500967264)
			Ni(0.728317201,0.500152886,0.499484032)
			Ni(0.271683276,0.500151813,0.499486476)
			C(0.999999464,0.166292340,0.501805305)
			C(0.999999642,0.333707482,0.501805186)
			C(0.500000894,0.416461289,0.497697532)
			C(0.500000656,0.083538584,0.497697949)
			C(0.891928256,0.419320762,0.501753926)
			C(0.108071022,0.080680028,0.501751304)
			C(0.108071290,0.419319898,0.501751125)
			C(0.891927958,0.080679044,0.501754224)
			C(0.390948355,0.168553427,0.497666687)
			C(0.609053314,0.331446409,0.497666031)
			C(0.609053135,0.168553755,0.497666299)
			C(0.390948385,0.331446141,0.497666508)
			C(0.000000646,0.666354775,0.501724362)
			C(0.000000463,0.833645344,0.501724482)
			C(0.500000358,0.915201426,0.498624623)
			C(0.500000536,0.584798515,0.498624206)
			C(0.891792893,0.919083238,0.501705348)
			C(0.108207896,0.580915928,0.501702189)
			C(0.108207680,0.919084191,0.501702368)
			C(0.891793132,0.580916703,0.501704991)
			C(0.391524702,0.668698967,0.499025375)
			C(0.608476102,0.831300855,0.499024659)
			C(0.608476162,0.668698788,0.499024391)
			C(0.391524762,0.831301153,0.499025583)
			Li1(0.499998927,0.250000894,0.556769967)

Table S3. Structural information of the optimized $Ni_8C_{24}Li2$.

Phase	Space Group	Lattice Parameters (Å, º)	Coordinates
$Ni_8C_{24}Li2$	PM	a =11.26964	Ni(0.228064358,0.249735832,0.500393212)
		b =8.69373	Ni(0.728567302,0.000000000,0.503117263)
		c=30.00000	Ni(0.773123026,0.250711799,0.502748132)
		α=β=γ=90.00000	Ni(0.272560865,0.999999583,0.500749350)
			Ni(0.228065088,0.750263810,0.500391603)
			Ni(0.730925381,0.499999881,0.491804838)
			Ni(0.773122430,0.749287963,0.502748549)
			Ni(0.272244811,0.500000060,0.501322925)
			C(0.000607229,0.166130796,0.501904070)
			C(0.499013156,0.415492445,0.498733073)
			C(0.000949154,0.333489865,0.501136422)
			C(0.501506448,0.084203027,0.500652671)
			C(0.892877936,0.419027239,0.500603437)
			C(0.392645627,0.168087229,0.500621259)
			C(0.108817779,0.080933623,0.501512825)
			C(0.608775377,0.332485139,0.498448819)
			C(0.108837321,0.419163704,0.501125813)
			C(0.609253824,0.169666544,0.500272155)
			C(0.892248094,0.081023581,0.503008962)
			C(0.391234428,0.329859257,0.500267863)
			C(0.000946653,0.666510284,0.501136243)
			C(0.501506686,0.915797532,0.500652671)
			C(0.000604604,0.833868802,0.501903832)
			C(0.499013424,0.584506750,0.498732954)
			C(0.892248571,0.918976367,0.503008962)
			C(0.391233504,0.670139849,0.500267625)
			C(0.108838595,0.580836058,0.501125515)
			C(0.609254241,0.830334485,0.500272155)
			C(0.108819164,0.919066489,0.501512527)
			C(0.608775735,0.667514026,0.498448670)
			C(0.892878294,0.580972493,0.500603378)
			C(0.392644882,0.831913650,0.500621021)
			Li2(0.609796107,0.500001848,0.557850420)

Table S4. Structural information of the optimized $Ni_8C_{24}Li3$.

Phase	Space Group	Lattice Parameters (Å, º)	Coordinates
$Ni_8C_{24}Li3$	PM	a =11.22601	Ni(0.230067834,0.260079354,0.502708912)
		b =8.66353	Ni(0.726903260,0.000000000,0.501987994)
		c=30.00000	Ni(0.771959424,0.249827906,0.503357530)
		α=β=γ=90.00000	Ni(0.269428283,0.000000000,0.501797676)
			Ni(0.230067834,0.739920616,0.502708912)
			Ni(0.728111207,0.500000000,0.504167199)

			Ni(0.771959424,0.750172079,0.503357530)
			Ni(0.276092142,0.500000000,0.473255306)
			C(0.000929923,0.166988686,0.504648805)
			C(0.498356730,0.416212022,0.500209272)
			C(0.000657225,0.334370792,0.504233539)
			C(0.499097914,0.083998099,0.496816278)
			C(0.892589450,0.418844521,0.504271328)
			C(0.390346587,0.168005347,0.495685488)
			C(0.108888842,0.080718577,0.505208313)
			C(0.607145965,0.331743985,0.501843452)
			C(0.111446865,0.418894976,0.504109919)
			C(0.607253432,0.169493392,0.499954522)
			C(0.891922057,0.081235453,0.504164100)
			C(0.390892982,0.330647260,0.495429546)
			C(0.000657225,0.665629208,0.504233539)
			C(0.499097914,0.916001916,0.496816278)
			C(0.000929923,0.833011329,0.504648805)
			C(0.498356730,0.583787978,0.500209272)
			C(0.891922057,0.918764532,0.504164100)
			C(0.390892982,0.669352710,0.495429546)
			C(0.111446865,0.581104994,0.504109919)
			C(0.607253432,0.830506623,0.499954522)
			C(0.108888842,0.919281423,0.505208313)
			C(0.607145965,0.668256044,0.501843452)
			C(0.892589450,0.581155479,0.504271328)
			C(0.390346587,0.831994653,0.495685488)
			Li3(0.269679010,0.500000000,0.551209092)

Table S5. Structural information of the optimized $Ni_8C_{24}Li4$.

Phase	Space Group	Lattice Parameters (Å, º)	Coordinates
$Ni_8C_{24}Li4$	PMM2	a =11.25432	Ni(0.227505177,0.249796614,0.501999319)
		b =8.69335	Ni(0.727625310,0.000000000,0.502631903)
		c=30.00000	Ni(0.772494853,0.249796614,0.501999319)
		α=β=γ=90.00000	Ni(0.272374690,0.000000000,0.502631903)
			Ni(0.227505177,0.750203371,0.501999319)
			Ni(0.727755249,0.500000000,0.500641048)
			Ni(0.772494853,0.750203371,0.501999319)
			Ni(0.272244722,0.500000000,0.500641048)
			C(0.000000000,0.166272745,0.503012002)
			C(0.500000000,0.414962590,0.492653757)
			C(0.000000000,0.333667785,0.502807260)
			C(0.500000000,0.084364787,0.501471758)
			C(0.891703665,0.419133425,0.502664626)
			C(0.391684145,0.169290364,0.500848830)

			C(0.108412758,0.080948107,0.503018558)
			C(0.608706594,0.331730008,0.497663885)
			C(0.108296320,0.419133425,0.502664626)
			C(0.608315825,0.169290364,0.500848830)
			C(0.891587257,0.080948107,0.503018558)
			C(0.391293406,0.331730008,0.497663885)
			C(0.000000000,0.666332185,0.502807260)
			C(0.500000000,0.915635228,0.501471758)
			C(0.000000000,0.833727241,0.503012002)
			C(0.500000000,0.585037410,0.492653757)
			C(0.891587257,0.919051886,0.503018558)
			C(0.391293406,0.668269992,0.497663885)
			C(0.108296320,0.580866575,0.502664626)
			C(0.608315825,0.830709636,0.500848830)
			C(0.108412758,0.919051886,0.503018558)
			C(0.608706594,0.668269992,0.497663885)
			C(0.891703665,0.580866575,0.502664626)
			C(0.391684145,0.830709636,0.500848830)
			Li4(0.500000000,0.500000000,0.557184398)

Table S6. Structural information of the optimized $Ni_8C_{24}Na1$.

Phase	Space Group	Lattice Parameters (Å, º)	Coordinates
$Ni_8C_{24}Na1$	PMM2	a =11.24857	Ni(0.227209195,0.249999747,0.501839399)
		b =8.70576	Ni(0.772793710,0.250000179,0.501841426)
		c=30.00000	Ni(0.728184760,0.999929309,0.499055564)
		α=β=γ=90.00000	Ni(0.271816254,0.999928832,0.499054313)
			Ni(0.227963045,0.750000477,0.501650095)
			Ni(0.772039413,0.749999702,0.501651347)
			Ni(0.728184581,0.500070572,0.499054998)
			Ni(0.271815717,0.500071406,0.499054879)
			C(0.000001766,0.166288421,0.503189325)
			C(0.000001965,0.333711594,0.503189325)
			C(0.499999613,0.416330218,0.495772302)
			C(0.500000715,0.083669730,0.495772213)
			C(0.891774774,0.419208676,0.503112853)
			C(0.108228363,0.080792457,0.503111541)
			C(0.108228512,0.419207722,0.503111541)
			C(0.891774595,0.080791257,0.503112972)
			C(0.391046017,0.168676376,0.495833725)
			C(0.608954966,0.331323236,0.495834023)
			C(0.608955503,0.168677792,0.495834023)
			C(0.391045481,0.331322491,0.495833814)
			C(0.000001093,0.666303456,0.503085077)
			C(0.000000935,0.833696723,0.503085136)

			C(0.500000715,0.915495753,0.497097582)
			C(0.499999642,0.584504247,0.497097641)
			C(0.891686440,0.919133782,0.503031015)
			C(0.108316638,0.580866635,0.503029644)
			C(0.108316503,0.919133604,0.503029704)
			C(0.891686678,0.580866098,0.503030896)
			C(0.391523421,0.668817878,0.497865915)
			C(0.608477056,0.831181347,0.497866213)
			C(0.608476579,0.668817699,0.497866184)
			C(0.391523987,0.831183076,0.497865826)
			Na1(0.500001609,0.249999538,0.569579422)

Table S7. Structural information of the optimized $Ni_8C_{24}Na2$.

Phase	Space Group	Lattice Parameters (Å, º)	Coordinates
$Ni_8C_{24}Na1$	PM	a =11.21061	Ni(0.228634238,0.257433593,0.500731349)
		b =8.67609	Ni(0.726135552,0.000000000,0.502731502)
		c=30.00000	Ni(0.771006763,0.249920815,0.504634857)
		α=β=γ=90.00000	Ni(0.269234538,0.000000000,0.499281943)
			Ni(0.228634238,0.742566407,0.500731349)
			Ni(0.726789534,0.500000000,0.505925715)
			Ni(0.771006763,0.750079155,0.504634857)
			Ni(0.270335078,0.500000000,0.474819571)
			C(0.999906063,0.166856632,0.504790008)
			C(0.497195423,0.416024595,0.498677552)
			C(0.999770939,0.334339857,0.504388094)
			C(0.498843342,0.084000498,0.496205181)
			C(0.891574383,0.418966860,0.505606055)
			C(0.389971703,0.167714521,0.493533999)
			C(0.107995458,0.080724008,0.504325569)
			C(0.606063247,0.331923246,0.502108097)
			C(0.110326946,0.418878198,0.503015280)
			C(0.606613100,0.169768512,0.500369310)
			C(0.890908718,0.081141241,0.505288005)
			C(0.389988869,0.330279917,0.492601633)
			C(0.999770939,0.665660143,0.504388094)
			C(0.498843342,0.915999532,0.496205181)
			C(0.999906063,0.833143353,0.504790008)
			C(0.497195423,0.583975375,0.498677552)
			C(0.890908718,0.918858767,0.505288005)
			C(0.389988869,0.669720113,0.492601633)
			C(0.110326946,0.581121802,0.503015280)
			C(0.606613100,0.830231488,0.500369310)
			C(0.107995458,0.919275999,0.504325569)
			C(0.606063247,0.668076754,0.502108097)

			C(0.891574383,0.581033111,0.505606055)
			C(0.389971703,0.832285464,0.493533999)
			Na2(0.303231299,0.500000000,0.562390625)

Table S8. Structural information of the optimized $Ni_8C_{24}Na3$.

Phase	Space Group	Lattice Parameters (Å, º)	Coordinates
$Ni_8C_{24}Na3$	PMM2	a =11.24064	Ni(0.227721557,0.249942705,0.502084613)
		b =8.69905	Ni(0.727711022,0.000000000,0.501210749)
		c=30.00000	Ni(0.772278488,0.249942705,0.502084613)
		α=β=γ=90.00000	Ni(0.272288978,0.000000000,0.501210749)
			Ni(0.227721557,0.750057280,0.502084613)
			Ni(0.727729559,0.500000000,0.499087453)
			Ni(0.772278488,0.750057280,0.502084613)
			Ni(0.272270441,0.500000000,0.499087453)
			C(0.000000000,0.166284591,0.503957212)
			C(0.500000000,0.415164024,0.490704328)
			C(0.000000000,0.333689570,0.503765702)
			C(0.500000000,0.084253021,0.499402404)
			C(0.891617656,0.419151962,0.503537178)
			C(0.391645253,0.169298977,0.498653769)
			C(0.108455494,0.080925561,0.503884435)
			C(0.608633041,0.331442803,0.495280981)
			C(0.108382344,0.419151962,0.503537178)
			C(0.608354747,0.169298977,0.498653769)
			C(0.891544521,0.080925561,0.503884435)
			C(0.391366959,0.331442803,0.495280981)
			C(0.000000000,0.666310430,0.503765702)
			C(0.500000000,0.915746987,0.499402404)
			C(0.000000000,0.833715379,0.503957212)
			C(0.500000000,0.584836006,0.490704328)
			C(0.891544521,0.919074416,0.503884435)
			C(0.391366959,0.668557227,0.495280981)
			C(0.108382344,0.580848038,0.503537178)
			C(0.608354747,0.830701053,0.498653769)
			C(0.108455494,0.919074416,0.503884435)
			C(0.608633041,0.668557227,0.495280981)
			C(0.891617656,0.580848038,0.503537178)
			C(0.391645253,0.830701053,0.498653769)
			Na3(0.500000000,0.500000000,0.567679644)

Table S9. Structural information of the optimized NiC_3Li.

Phase	Space Group	Lattice Parameters (Å, º)	Coordinates
NiC_3Li	CMMM	a =11.68329	Ni(0.223750994,0.499996990,0.500000000)

	b =4.30701	Ni(0.776247025,0.499994010,0.500000000)
	c=30.00000	Ni(0.723752975,0.000007000,0.500000000)
	α=β=γ=90.00000	Ni(0.276248991,0.000003000,0.500000000)
		C(0.999998987,0.330859989,0.500000000)
		C(0.999998987,0.669139981,0.500000000)
		C(0.500001013,0.830860019,0.500000000)
		C(0.500001013,0.169139996,0.500000000)
		C(0.890263021,0.831768990,0.500000000)
		C(0.109734997,0.168228000,0.500000000)
		C(0.109734997,0.831772029,0.500000000)
		C(0.890263021,0.168231994,0.500000000)
		C(0.390264988,0.331772000,0.500000000)
		C(0.609736979,0.668231010,0.500000000)
		C(0.609736979,0.331768006,0.500000000)
		C(0.390264988,0.668227971,0.500000000)
		Li(0.499998987,0.500000000,0.556143999)
		Li(0.499998987,0.500000000,0.443856001)
		Li(0.000002000,0.000000000,0.556143999)
		Li(0.000002000,0.000000000,0.443856001)

Table S10. Structural information of the optimized NiC_3Li_3.

Phase	Space Group	Lattice Parameters (Å, º)	Coordinates
NiC_3Li_3	CMMM	a =12.03793	Ni(0.222685993,0.500000000,0.500000000)
		b =4.28398	Ni(0.777310014,0.500000000,0.500000000)
		c=30.00000	Ni(0.722684979,0.000000000,0.500000000)
		α=β=γ=90.00000	Ni(0.277310014,0.000000000,0.500000000)
			C(0.999998987,0.330249995,0.500000000)
			C(0.999998987,0.669749975,0.500000000)
			C(0.500000000,0.830247998,0.500000000)
			C(0.500000000,0.169752002,0.500000000)
			C(0.891326010,0.831224024,0.500000000)
			C(0.108678997,0.168792993,0.500000000)
			C(0.108678997,0.831206977,0.500000000)
			C(0.891326010,0.168776006,0.500000000)
			C(0.391319990,0.331256986,0.500000000)
			C(0.608678997,0.668752015,0.500000000)
			C(0.608678997,0.331247985,0.500000000)
			C(0.391319990,0.668743014,0.500000000)
			Li(0.500002980,0.500000000,0.558749020)
			Li(0.500002980,0.500000000,0.441251010)
			Li(0.000000000,0.000000000,0.558749974)
			Li(0.000000000,0.000000000,0.441249996)
			Li(0.120278001,0.500000000,0.565339029)

			Li(0.879718006,0.500000000,0.434666008)
			Li(0.879718006,0.500000000,0.565334022)
			Li(0.120278001,0.500000000,0.434661001)
			Li(0.620278001,0.000000000,0.565339029)
			Li(0.379723996,0.000000000,0.434664011)
			Li(0.379723996,0.000000000,0.565335989)
			Li(0.620278001,0.000000000,0.434661001)

Table S11. Structural information of the optimized NiC_3Li_4.

Phase	Space Group	Lattice Parameters (Å, º)	Coordinates
NiC_3Li_4	CMMM	a =11.95563	Ni(0.222442001,0.499994993,0.500001013)
		b =4.26056	Ni(0.777513981,0.499998987,0.500000000)
		c=30.00000	Ni(0.722443998,0.000003000,0.500001013)
		α=β=γ=90.00000	Ni(0.277514994,0.000000000,0.499998987)
			C(0.999979973,0.329959005,0.500000000)
			C(0.999979973,0.670041025,0.500000000)
			C(0.499980986,0.829958975,0.500000000)
			C(0.499980003,0.170040995,0.500000000)
			C(0.890823007,0.830388010,0.500000000)
			C(0.109136999,0.169605002,0.500001013)
			C(0.109136999,0.830394030,0.500001013)
			C(0.890823007,0.169613004,0.500000000)
			C(0.390823007,0.330388010,0.499998987)
			C(0.609138012,0.669605970,0.500001013)
			C(0.609138012,0.330394000,0.500001013)
			C(0.390823007,0.669613004,0.499998987)
			Li(0.500000000,0.500000000,0.556896985)
			Li(0.500003994,0.500000000,0.443102986)
			Li(0.000003000,0.000000000,0.556896985)
			Li(0.000006000,0.000000000,0.443102986)
			Li(0.499996006,0.500000000,0.640994012)
			Li(0.499996990,0.500000000,0.359005004)
			Li(0.999997973,0.000000000,0.640995026)
			Li(0.999998987,0.000000000,0.359005004)
			Li(0.123011000,0.500000000,0.568217993)
			Li(0.877072990,0.500000000,0.431807995)
			Li(0.877071023,0.500000000,0.568192005)
			Li(0.123014003,0.500000000,0.431782991)
			Li(0.623004973,0.000001000,0.568216026)
			Li(0.377068996,0.000001000,0.431805998)
			Li(0.377065986,0.000001000,0.568193018)
			Li(0.623008013,0.000001000,0.431784987)

Table S12. Structural information of the optimized NiC_3Li_6.

Phase	Space Group	Lattice Parameters (Å, º)	Coordinates
NiC_3Li_6	CMMM	a =11.80220	Ni(0.223885000,0.500000000,0.500000000)
		b =4.26998	Ni(0.776115000,0.500000000,0.500000000)
		c=30.00000	Ni(0.723887026,0.000000000,0.500000000)
		α=β=γ=90.00000	Ni(0.276113003,0.000000000,0.500000000)
			C(0.000000000,0.330228001,0.500000000)
			C(0.000000000,0.669772029,0.500000000)
			C(0.500000000,0.830226004,0.500000000)
			C(0.500000000,0.169773996,0.500000000)
			C(0.890614986,0.831497014,0.500000000)
			C(0.109384999,0.168503001,0.500000000)
			C(0.109384999,0.831497014,0.500000000)
			C(0.890614986,0.168503001,0.500000000)
			C(0.390612006,0.331485003,0.500000000)
			C(0.609387994,0.668515027,0.500000000)
			C(0.609387994,0.331485003,0.500000000)
			C(0.390612006,0.668515027,0.500000000)
			Li(0.500000000,0.500000000,0.559924006)
			Li(0.500000000,0.500000000,0.440075994)
			Li(0.000000000,0.000000000,0.559924006)
			Li(0.000000000,0.000000000,0.440075994)
			Li(0.500000000,0.500000000,0.644650996)
			Li(0.500000000,0.500000000,0.355349004)
			Li(0.000000000,0.000000000,0.644649982)
			Li(0.000000000,0.000000000,0.355349988)
			Li(0.125532001,0.500000000,0.567294002)
			Li(0.874468029,0.500000000,0.432705998)
			Li(0.874468029,0.500000000,0.567294002)
			Li(0.125532001,0.500000000,0.432705998)
			Li(0.625533998,0.000000000,0.567296028)
			Li(0.374466002,0.000000000,0.432704002)
			Li(0.374466002,0.000000000,0.567296028)
			Li(0.625533998,0.000000000,0.432704002)
			Li(0.165058002,0.500000000,0.652738988)
			Li(0.834941983,0.500000000,0.347261012)
			Li(0.834941983,0.500000000,0.652738988)
			Li(0.165058002,0.500000000,0.347261012)
			Li(0.665058970,0.000000000,0.652738988)
			Li(0.334941000,0.000000000,0.347261012)
			Li(0.334941000,0.000000000,0.652738988)
			Li(0.665058970,0.000000000,0.347261012)

Table S13. Structural information of the optimized NiC_3Na_2.

Phase	Space Group	Lattice Parameters (Å, º)	Coordinates
NiC_3Na_2	CMMM	a =11.80939	Ni(0.225899220,0.500004530,0.499999464)
		b =4.24588	Ni(0.774089515,0.499997944,0.500000775)
		c=30.00000	Ni(0.725908518,0.000001686,0.499999374)
		α=β=γ=90.00000	Ni(0.274099678,0.999996245,0.500000417)
			C(0.999998152,0.328540921,0.500000000)
			C(0.999998093,0.671458840,0.500000000)
			C(0.500000119,0.828541338,0.499999970)
			C(0.500000060,0.171458811,0.499999970)
			C(0.892639637,0.832497597,0.500000417)
			C(0.107354231,0.167494327,0.499999702)
			C(0.107354283,0.832504988,0.499999702)
			C(0.892639637,0.167502642,0.500000417)
			C(0.392643005,0.332506180,0.500000179)
			C(0.607358575,0.667502344,0.499999672)
			C(0.607358515,0.332497388,0.499999672)
			C(0.392643005,0.667494476,0.500000179)
			Na(0.126364648,0.499999791,0.579469860)
			Na(0.873647571,0.500000060,0.420527011)
			Na(0.873649478,0.500000060,0.579473972)
			Na(0.126363263,0.499999821,0.420529544)
			Na(0.626356125,0.000000000,0.579473794)
			Na(0.373639554,0.000000142,0.420530707)
			Na(0.373640716,0.000000124,0.579469681)
			Na(0.626354516,0.000000000,0.420525491)

Table S14. Structural information of the optimized NiC_3Na_3.

Phase	Space Group	Lattice Parameters (Å, º)	Coordinates
NiC_3Na_3	CMMM	a =11.77726	Ni(0.226296946,0.500000000,0.499994516)
		b =4.25216	Ni(0.773704469,0.500000000,0.500005484)
		c=30.00000	Ni(0.726295948,0.000000000,0.499994516)
		α=β=γ=90.00000	Ni(0.273702502,0.000000000,0.500005543)
			C(0.000000371,0.328729242,0.500000000)
			C(0.000000371,0.671270728,0.500000000)
			C(0.499999166,0.828729331,0.500000000)
			C(0.499999166,0.171270683,0.500000000)
			C(0.892489612,0.832676649,0.500003159)
			C(0.107513353,0.167328730,0.499996871)
			C(0.107513353,0.832671285,0.499996871)
			C(0.892489612,0.167323351,0.500003159)
			C(0.392486125,0.332671493,0.500003159)
			C(0.607509911,0.667323232,0.499996841)
			C(0.607509911,0.332676768,0.499996841)

			C(0.392486125,0.667328477,0.500003159)
			Na(0.127716675,0.500000000,0.579456449)
			Na(0.872274816,0.499999970,0.420548886)
			Na(0.872285187,0.500000000,0.579457223)
			Na(0.127706319,0.499999970,0.420537531)
			Na(0.627725184,0.000000000,0.579451323)
			Na(0.372283369,0.000000000,0.420544356)
			Na(0.372293741,0.000000000,0.579461694)
			Na(0.627714753,0.000000000,0.420542568)
			Na(0.500010133,0.500000000,0.656147122)
			Na(0.500003576,0.499999970,0.343852848)
			Na(0.999997914,0.000000000,0.656147063)
			Na(0.999991417,0.000000000,0.343852967)

Table S15. Structural information of the optimized NiC_3Na_5.

Phase	Space Group	Lattice Parameters (Å, º)	Coordinates
NiC_3Na_5	CMMM	a =11.80587	Ni(0.226274595,0.500000000,0.499981582)
		b =4.25146	Ni(0.773730218,0.500000298,0.500018775)
		c=30.00000	Ni(0.726269841,0.000000281,0.499981374)
		α=β=γ=90.00000	Ni(0.273725390,0.000000000,0.500018299)
			C(0.000001920,0.328724027,0.500000060)
			C(0.000001924,0.671276271,0.500000060)
			C(0.499998093,0.828724027,0.499999970)
			C(0.499998093,0.171276271,0.499999970)
			C(0.892642558,0.832587481,0.500010371)
			C(0.107360765,0.167413145,0.499989718)
			C(0.107360773,0.832587123,0.499989718)
			C(0.892642558,0.167412773,0.500010371)
			C(0.392639220,0.332587034,0.500010252)
			C(0.607357502,0.667412817,0.499989688)
			C(0.607357502,0.332587630,0.499989688)
			C(0.392639250,0.667413056,0.500010252)
			Na(0.130208582,0.500000536,0.579668045)
			Na(0.869784474,0.499999315,0.420336813)
			Na(0.869827807,0.499999315,0.579684496)
			Na(0.130165294,0.500000477,0.420310795)
			Na(0.630215943,0.000000691,0.579663098)
			Na(0.369791299,0.999999166,0.420331925)
			Na(0.369834214,0.999999166,0.579689085)
			Na(0.630172968,0.000000687,0.420315713)
			Na(0.500019193,0.499999881,0.650469542)
			Na(0.499985665,0.499999881,0.349530369)
			Na(0.000014327,0.999999881,0.650469661)
			Na(0.999980867,0.999999881,0.349530369)

			Na(0.645401895,0.999999702,0.710660875)
			Na(0.354598373,0.000000000,0.289338768)
			Na(0.354604155,0.000000000,0.710660875)
			Na(0.645396054,0.999999702,0.289339304)
			Na(0.145401642,0.499999702,0.710660994)
			Na(0.854597747,0.500000000,0.289339244)
			Na(0.854603589,0.500000000,0.710660577)
			Na(0.145395815,0.499999702,0.289339215)

Table S16. Structural information of the optimized NiC_3Na_6.

Phase	Space Group	Lattice Parameters (Å, º)	Coordinates
NiC_3Na_6	PMMM	a =11.91986	Ni(0.221774653,0.500000000,0.500000000)
		b =4.27978	Ni(0.778225362,0.500000000,0.500000000)
		c=30.00000	Ni(0.724278033,0.000000000,0.500000000)
		α=β=γ=90.00000	Ni(0.275721997,0.000000000,0.500000000)
			C(0.000000000,0.329684734,0.500000000)
			C(0.000000000,0.670315266,0.500000000)
			C(0.500000000,0.829572260,0.500000000)
			C(0.500000000,0.170427755,0.500000000)
			C(0.892983556,0.832463861,0.500000000)
			C(0.107016459,0.167536139,0.500000000)
			C(0.107016459,0.832463861,0.500000000)
			C(0.892983556,0.167536139,0.500000000)
			C(0.392143548,0.332144469,0.500000000)
			C(0.607856452,0.667855561,0.500000000)
			C(0.607856452,0.332144469,0.500000000)
			C(0.392143548,0.667855561,0.500000000)
			Na(0.166967109,0.500000000,0.590518355)
			Na(0.833032906,0.500000000,0.409481615)
			Na(0.833032906,0.500000000,0.590518355)
			Na(0.166967109,0.500000000,0.409481615)
			Na(0.649626315,0.000000000,0.582257211)
			Na(0.350373685,0.000000000,0.417742789)
			Na(0.350373685,0.000000000,0.582257211)
			Na(0.649626315,0.000000000,0.417742789)
			Na(0.150063574,0.500000000,0.753768802)
			Na(0.849936426,0.500000000,0.246231228)
			Na(0.849936426,0.500000000,0.753768802)
			Na(0.150063574,0.500000000,0.246231228)
			Na(0.722573042,0.000000000,0.680903614)
			Na(0.277426928,0.000000000,0.319096386)
			Na(0.277426928,0.000000000,0.680903614)
			Na(0.722573042,0.000000000,0.319096386)
			Na(0.500000000,0.500000000,0.575065911)

	Na(0.500000000,0.500000000,0.424934089)
	Na(0.000000000,0.000000000,0.574231327)
	Na(0.000000000,0.000000000,0.425768644)
	Na(0.500000000,0.500000000,0.681591749)
	Na(0.500000000,0.500000000,0.318408281)
	Na(0.000000000,0.000000000,0.678954422)
	Na(0.000000000,0.000000000,0.321045578)