Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Electronic Supplementary Information

A Data-driven Interpretable Method to Predict Capacities of Metal ion Doped TiO_2 Anode Materials for Lithium-ion Batteries Using Machine Learning Classifiers

Mingxi Jiang [a], Yajuan Zhang [a], Zihao Yang [a], Haibo Li [b], Jinliang Li [c], Jiabao Li [d], Ting Lu [a], Chenglong Wang [a,*], Guang Yang [a,*], Likun Pan [a,*]

[a] *Shanghai Key Laboratory of Magnetic Resonance, School of Physics and Electronic Science, East China Normal University, Shanghai 200241, China*

[b] *Ningxia Key Laboratory of Photovoltaic Materials, School of Materials and New Energy, Ningxia University, Yinchuan 750021, China*

[c] *Siyuan Laboratory, Guangdong Provincial Engineering Technology Research Center of Vacuum Coating Technologies and New Energy Materials, Department of Physics, Jinan University, Guangzhou 510632, China*

[d] *School of Chemistry and Chemical Engineering, Yangzhou University, Yangzhou, Jiangsu 225002, China*

**Corresponding authors*

E-mail addresses: lkpan@phy.ecnu.edu.cn *(Likun Pan);* clwang@phy.ecnu.edu.cn *(Chenglong Wang);* gyang@phy.ecnu.edu.cn *(Guang Yang)*

Supplementary Table S1. Datasets: electronegativity of the doped elements (en), atom ratio of dopant and Ti (ratio), dopant's ionic radius (radius), state of the dopant (state), material molecule mass (Mweight), molecule single bond covalent radius (rc), bond formation enthalpy of doped element and oxygen (feo), current density (current), lowest potential during charging and discharging (low), highest potential during charging and discharging (high), capacity values at different current densities (capacity).

elements	en	ratio	radius (nm)	state	rc (nm)	feo (KJ)	Mweight	low (V)	high (V)	current (A/ g)	capacity (mAh/ g)	Ref
Mg	1.31	0.02	0.072	2	1.39	601.6	79.428	0.8	2.8	0.0167	160	1
Mg	1.31	0.02	0.072	2	1.39	601.6	79.428	0.8	2.8	0.084	155	1
Mg	1.31	0.02	0.072	2	1.39	601.6	79.428	0.8	2.8	0.167	140	1
Mg	1.31	0.02	0.072	2	1.39	601.6	79.428	0.8	2.8	0.335	123	1
Mg	1.31	0.02	0.072	2	1.39	601.6	79.428	0.8	2.8	0.835	95	1
Mg	1.31	0.01	0.072	2	1.39	601.6	79.664	0.8	2.8	0.0167	163	1
Mg	1.31	0.01	0.072	2	1.39	601.6	79.664	0.8	2.8	0.084	152	1
Mg	1.31	0.01	0.072	2	1.39	601.6	79.664	0.8	2.8	0.167	136	1
Mg	1.31	0.01	0.072	2	1.39	601.6	79.664	0.8	2.8	0.335	115d	1
Mg	1.31	0.01	0.072	2	1.39	601.6	79.664	0.8	2.8	0.835	80	1
Mg	1.31	0.04	0.072	2	1.39	601.6	78.956	0.8	2.8	0.0167	159	1
Mg	1.31	0.04	0.072	2	1.39	601.6	78.956	0.8	2.8	0.084	139	1
Mg	1.31	0.04	0.072	2	1.39	601.6	78.956	0.8	2.8	0.167	110	1
Mg	1.31	0.04	0.072	2	1.39	601.6	78.956	0.8	2.8	0.335	82	1
Mg	1.31	0.04	0.072	2	1.39	601.6	78.956	0.8	2.8	0.835	50	1
Sn	1.96	0.03	0.069	4	1.4	290.4	82.024	1	3	0.0167	266	2
Sn	1.96	0.05	0.069	4	1.4	290.4	83.44	1	3	0.0167	342	2
Sn	1.96	0.05	0.069	4	1.4	290.4	83.44	1	3	0.0335	325	2
Sn	1.96	0.05	0.069	4	1.4	290.4	83.44	1	3	0.167	295	2
Sn	1.96	0.05	0.069	4	1.4	290.4	83.44	1	3	0.335	260	2
Sn	1.96	0.05	0.069	4	1.4	290.4	83.44	1	3	0.835	206	2
Sn	1.96	0.07	0.069	4	1.4	290.4	84.856	1	3	0.0167	207	2
Nb	1.6	0.25	0.064	5	1.47	379.9	91.15	1.2	3	0.5	162	3
Nb	1.6	0.25	0.064	5	1.47	379.9	91.15	1.2	3	2	136	3
Nb	1.6	0.25	0.064	5	1.47	379.9	91.15	1.2	3	5	100	3
Nb	1.6	0.25	0.064	5	1.47	379.9	91.15	1.2	3	0.1	180	3

Nb	1.6	0.25	0.064	5	1.47	379.9	91.15	1.2	3	1	150	3
Nb	1.6	0.25	0.064	5	1.47	379.9	91.15	1.2	3	10	75	3
Sn	1.96	0.1	0.069	4	1.47	290.4	86.98	0.1	3	0.1	300	4
Sn	1.96	0.1	0.069	4	1.47	290.4	86.98	0.1	3	0.3	240	4
Sn	1.96	0.1	0.069	4	1.47	290.4	86.98	0.1	3	0.5	195	4
Sn	1.96	0.1	0.069	4	1.47	290.4	86.98	0.1	3	1	150	4
Fe	1.83	NAN	0.0645	3	1.16	549.5	80.46	0.01	3	0.335	160	5
Fe	1.83	NAN	0.0645	3	1.16	549.5	80.46	0.01	3	0.67	123	5
Fe	1.83	NAN	0.0645	3	1.16	549.5	80.46	0.01	3	1	123	5
Fe	1.83	NAN	0.0645	3	1.16	549.5	80.46	0.01	3	1.67	103	5
Fe	1.83	NAN	0.0645	3	1.16	549.5	80.46	0.01	3	3.35	75	5
Fe	1.83	NAN	0.0645	3	1.16	549.5	80.46	0.01	3	6.7	58	5
Ti	1.54	0.05	0.067	3	1.36	1012	79.9	1	3	0.17	195	6
Ti	1.54	0.05	0.067	3	1.36	1012	79.9	1	3	1.7	103	6
Ti	1.54	0.05	0.067	3	1.36	1012	79.9	1	3	6.8	50	6
Nb	1.6	0.04	0.069	5	1.47	379.9	81.7	0.5	3	0.25	296	7
Nb	1.6	0.04	0.069	5	1.47	379.9	81.7	0.5	3	1	237	7
Nb	1.6	0.04	0.069	5	1.47	379.9	81.7	0.5	3	0.05	360	7
Nb	1.6	0.04	0.069	5	1.47	379.9	81.7	0.5	3	0.5	265	7
Ni	1.91	0.0245	0.069	2	1.1	239.7	80.1646	0.05	3	0.1	145	8
Ni	1.91	0.0245	0.069	2	1.1	239.7	80.1646	0.05	3	1	82	8
Ni	1.91	0.0245	0.069	2	1.1	239.7	80.1646	0.05	3	0.04	185	8
Ni	1.91	0.0245	0.069	2	1.1	239.7	80.1646	0.05	3	0.2	100	8
Ni	1.91	0.0245	0.069	2	1.1	239.7	80.1646	0.05	3	0.4	80	8
Ni	1.91	0.008	0.069	2	1.1	239.7	79.9864	0.05	3	0.1	105	8
Ni	1.91	0.008	0.069	2	1.1	239.7	79.9864	0.05	3	1	45	8
Ni	1.91	0.008	0.069	2	1.1	239.7	79.9864	0.05	3	0.04	150	8
Ni	1.91	0.008	0.069	2	1.1	239.7	79.9864	0.05	3	0.2	90	8
Ni	1.91	0.008	0.069	2	1.1	239.7	79.9864	0.05	3	0.4	60	8
Mn	1.55	0.1	0.054	4	1.19	519.7	80.6	1	3	0.0167	130	9
Mn	1.55	0.1	0.054	4	1.19	519.7	80.6	1	3	0.084	110	9
Mn	1.55	0.1	0.054	4	1.19	519.7	80.6	1	3	0.335	60	9
Mn	1.55	0.2	0.054	4	1.19	519.7	81.3	1	3	0.0167	123	9
Mn	1.55	0.2	0.054	4	1.19	519.7	81.3	1	3	0.084	100	9
Mn	1.55	0.2	0.054	4	1.19	519.7	81.3	1	3	0.335	42	9
Sn	1.96	0.06	0.069	4	1.4	290.4	84.148	0.01	3	0.084	270	10
Sn	1.96	0.06	0.069	4	1.4	290.4	84.148	0.01	3	0.167	180	10
Sn	1.96	0.06	0.069	4	1.4	290.4	84.148	0.01	3	0.0167	300	10
Sn	1.96	0.06	0.069	4	1.4	290.4	84.148	0.01	3	0.0335	240	10

Mn	1.55	0.05	0.054	4	1.19	519.7	80.25	1	3	0.0167	190	9
Mn	1.55	0.05	0.054	4	1.19	519.7	80.25	1	3	0.084	165	9
Mn	1.55	0.05	0.054	4	1.19	519.7	80.25	1	3	0.335	125	9
Cu	1.9	0.0355	0.073	2	1.12	157.3	80.45735	1	3.2	0.335	170	11
Cu	1.9	0.0355	0.073	2	1.12	157.3	80.45735	1	3.2	3.34	130	11
Cu	1.9	0.0355	0.073	2	1.12	157.3	80.45735	1	3.2	8.35	98	11
Cu	1.9	0.0355	0.073	2	1.12	157.3	80.45735	1	3.2	0.67	170	11
Cu	1.9	0.0355	0.073	2	1.12	157.3	80.45735	1	3.2	6.7	125	11
Cu	1.9	0.067	0.073	2	1.12	157.3	80.9519	1	3.2	0.335	175	11
Cu	1.9	0.067	0.073	2	1.12	157.3	80.9519	1	3.2	3.34	160	11
Cu	1.9	0.067	0.073	2	1.12	157.3	80.9519	1	3.2	8.35	130	11
Cu	1.9	0.067	0.073	2	1.12	157.3	80.9519	1	3.2	0.67	175	11
Cu	1.9	0.067	0.073	2	1.12	157.3	80.9519	1	3.2	6.7	152	11
Cu	1.9	0.095	0.073	2	1.12	157.3	81.3915	1	3.2	0.335	165	11
Cu	1.9	0.095	0.073	2	1.12	157.3	81.3915	1	3.2	3.34	117	11
Cu	1.9	0.095	0.073	2	1.12	157.3	81.3915	1	3.2	8.35	80	11
Cu	1.9	0.095	0.073	2	1.12	157.3	81.3915	1	3.2	0.67	169	11
Cu	1.9	0.095	0.073	2	1.12	157.3	81.3915	1	3.2	6.7	119	11
Mn	1.55	0.04	0.067	2	1.19	519.7	80.18	1	2.5	0.03	90	12
Mn	1.55	0.04	0.067	2	1.19	519.7	80.18	1	2.5	0.5	26	12
Mn	1.55	0.04	0.067	2	1.19	519.7	80.18	1	2.5	0.15	50	12
Ni	1.91	0.07	0.069	2	1.1	239.7	80.656	1	2.5	0.03	223	12
Ni	1.91	0.07	0.069	2	1.1	239.7	80.656	1	2.5	0.5	156	12
Ni	1.91	0.07	0.069	2	1.1	239.7	80.656	1	2.5	0.15	200	12
Cu	1.9	0.0255	0.073	2	1.12	157.3	80.30035	1	3	0.167	216	13
Cu	1.9	0.0255	0.073	2	1.12	157.3	80.30035	1	3	1.67	170	13
Cu	1.9	0.0255	0.073	2	1.12	157.3	80.30035	1	3	5	127	13
Cu	1.9	0.0255	0.073	2	1.12	157.3	80.30035	1	3	10	103	13
Cu	1.9	0.0255	0.073	2	1.12	157.3	80.30035	1	3	0.084	250	13
Cu	1.9	0.0255	0.073	2	1.12	157.3	80.30035	1	3	2.5	170	13
Cu	1.9	0.0255	0.073	2	1.12	157.3	80.30035	1	3	3.35	150	13
Cr	1.66	0.05	0.0615	3	1.22	756.5	80.105	1	3	0.167	145	14
Cr	1.66	0.05	0.0615	3	1.22	756.5	80.105	1	3	0.084	190	14
Cr	1.66	0.05	0.0615	3	1.22	756.5	80.105	1	3	0.835	100	14
Cr	1.66	0.05	0.0615	3	1.22	756.5	80.105	1	3	0.335	125	14
Co	1.88	0.025	0.065	2	1.11	606.6	80.175	0.01	3	0.0335	175	15
Co	1.88	0.025	0.065	2	1.11	606.6	80.175	0.01	3	0.067	146	15
Co	1.88	0.025	0.065	2	1.11	606.6	80.175	0.01	3	0.167	98	15
Co	1.88	0.025	0.065	2	1.11	606.6	80.175	0.01	3	0.335	90	15

Co	1.88	0.025	0.065	2	1.11	606.6	80.175	0.01	3	0.67	70	15
Co	1.88	0.042	0.065	2	1.11	606.6	80.362	0.01	3	0.0335	180	15
Co	1.88	0.042	0.065	2	1.11	606.6	80.362	0.01	3	0.067	150	15
Co	1.88	0.042	0.065	2	1.11	606.6	80.362	0.01	3	0.167	95	15
Co	1.88	0.042	0.065	2	1.11	606.6	80.362	0.01	3	0.335	80	15
Co	1.88	0.042	0.065	2	1.11	606.6	80.362	0.01	3	0.67	50	15
Co	1.88	0.058	0.065	2	1.11	606.6	80.538	0.01	3	0.0335	200	15
Co	1.88	0.058	0.065	2	1.11	606.6	80.538	0.01	3	0.067	176	15
Co	1.88	0.058	0.065	2	1.11	606.6	80.538	0.01	3	0.167	150	15
Co	1.88	0.058	0.065	2	1.11	606.6	80.538	0.01	3	0.335	116	15
Co	1.88	0.058	0.065	2	1.11	606.6	80.538	0.01	3	0.67	96	15
Sn	1.96	0.017	0.069	4	1.4	290.4	81.1036	0	3	0.05	245	16
Sn	1.96	0.017	0.069	4	1.4	290.4	81.1036	0	3	0.25	150	16
Sn	1.96	0.017	0.069	4	1.4	290.4	81.1036	0	3	1.25	105	16
Sn	1.96	0.017	0.069	4	1.4	290.4	81.1036	0	3	5	220	16
Nb	1.6	0.0237	0.069	5	1.47	379.9	80.9665	1	3	0.167	175	17
Nb	1.6	0.0237	0.069	5	1.47	379.9	80.9665	1	3	0.335	160	17
Nb	1.6	0.0237	0.069	5	1.47	379.9	80.9665	1	3	0.668	148	17
Nb	1.6	0.0237	0.069	5	1.47	379.9	80.9665	1	3	1.67	125	17
Nb	1.6	0.0237	0.069	5	1.47	379.9	80.9665	1	3	3.35	112	17
Nb	1.6	0.0237	0.069	5	1.47	379.9	80.9665	1	3	5	109	17
Nb	1.6	0.0644	0.069	5	1.47	379.9	82.798	1	3	0.167	190	17
Nb	1.6	0.0644	0.069	5	1.47	379.9	82.798	1	3	0.335	174	17
Nb	1.6	0.0644	0.069	5	1.47	379.9	82.798	1	3	0.668	160	17
Nb	1.6	0.0644	0.069	5	1.47	379.9	82.798	1	3	1.67	135	17
Nb	1.6	0.0644	0.069	5	1.47	379.9	82.798	1	3	3.35	126	17
Nb	1.6	0.0644	0.069	5	1.47	379.9	82.798	1	3	5	120	17
Nb	1.6	0.0976	0.069	5	1.47	379.9	84.292	1	3	0.167	210	17
Nb	1.6	0.0976	0.069	5	1.47	379.9	84.292	1	3	0.335	198	17
Nb	1.6	0.0976	0.069	5	1.47	379.9	84.292	1	3	0.668	180	17
Nb	1.6	0.0976	0.069	5	1.47	379.9	84.292	1	3	1.67	168	17
Nb	1.6	0.0976	0.069	5	1.47	379.9	84.292	1	3	3.35	147	17
Nb	1.6	0.0976	0.069	5	1.47	379.9	84.292	1	3	5	139	17
Nb	1.6	0.04	0.069	5	1.47	379.9	81.7	1	3	0.335	175	18
Nb	1.6	0.04	0.069	5	1.47	379.9	81.7	1	3	1.67	125	18
Nb	1.6	0.04	0.069	5	1.47	379.9	81.7	1	3	6.7	80	18
Nb	1.6	0.04	0.069	5	1.47	379.9	81.7	1	3	0.167	180	18
Nb	1.6	0.04	0.069	5	1.47	379.9	81.7	1	3	0.067	205	18
Nb	1.6	0.04	0.069	5	1.47	379.9	81.7	1	3	0.67	149	18

Nb	1.6	0.04	0.069	5	1.47	379.9	81.7	1	3	3.35	110	18
Nb	1.6	0.07	0.069	5	1.47	379.9	83.05	1	3	0.335	168	18
Nb	1.6	0.07	0.069	5	1.47	379.9	83.05	1	3	1.67	120	18
Nb	1.6	0.07	0.069	5	1.47	379.9	83.05	1	3	6.7	72	18
Nb	1.6	0.07	0.069	5	1.47	379.9	83.05	1	3	0.167	175	18
Nb	1.6	0.07	0.069	5	1.47	379.9	83.05	1	3	0.067	195	18
Nb	1.6	0.07	0.069	5	1.47	379.9	83.05	1	3	0.67	143	18
Nb	1.6	0.07	0.069	5	1.47	379.9	83.05	1	3	3.35	106	18
Nb	1.6	0.001	0.069	5	1.47	379.9	79.945	1	2.9	0.335	190	19
Nb	1.6	0.001	0.069	5	1.47	379.9	79.945	1	2.9	1.67	140	19
Nb	1.6	0.001	0.069	5	1.47	379.9	79.945	1	2.9	5	105	19
Nb	1.6	0.001	0.069	5	1.47	379.9	79.945	1	2.9	0.167	215	19
Nb	1.6	0.001	0.069	5	1.47	379.9	79.945	1	2.9	10	79	19
Nb	1.6	0.01	0.069	5	1.47	379.9	80.35	1	2.9	0.335	145	19
Nb	1.6	0.01	0.069	5	1.47	379.9	80.35	1	2.9	1.67	96	19
Nb	1.6	0.01	0.069	5	1.47	379.9	80.35	1	2.9	5	63	19
Nb	1.6	0.01	0.069	5	1.47	379.9	80.35	1	2.9	0.167	160	19
Nb	1.6	0.01	0.069	5	1.47	379.9	80.35	1	2.9	10	62	19
Nb	1.6	0.1	0.069	5	1.47	379.9	84.4	1	2.9	0.335	105	19
Nb	1.6	0.1	0.069	5	1.47	379.9	84.4	1	2.9	1.67	65	19
Nb	1.6	0.1	0.069	5	1.47	379.9	84.4	1	2.9	5	47	19
Nb	1.6	0.1	0.069	5	1.47	379.9	84.4	1	2.9	0.167	120	19
Nb	1.6	0.1	0.069	5	1.47	379.9	84.4	1	2.9	10	32	19
Cu	1.9	0.0233	0.073	2	1.12	157.3	80.26581	1	3	3.35	120	20
Cu	1.9	0.0233	0.073	2	1.12	157.3	80.26581	1	3	1.67	130	20
Cu	1.9	0.0233	0.073	2	1.12	157.3	80.26581	1	3	0.084	195	20
Cu	1.9	0.0233	0.073	2	1.12	157.3	80.26581	1	3	0.167	177	20
Cu	1.9	0.0233	0.073	2	1.12	157.3	80.26581	1	3	0.335	170	20
Sn	1.96	0.06	0.069	4	1.4	290.4	84.148	0.05	3	0.1	260	21
Sn	1.96	0.06	0.069	4	1.4	290.4	84.148	0.05	3	0.2	223	21
Sn	1.96	0.06	0.069	4	1.4	290.4	84.148	0.05	3	0.3	200	21
Sn	1.96	0.06	0.069	4	1.4	290.4	84.148	0.05	3	0.5	172	21
Sn	1.96	0.06	0.069	4	1.4	290.4	84.148	0.05	3	1	135	21
Sn	1.96	0.06	0.069	4	1.4	290.4	84.148	0.05	3	1.5	110	21
Sn	1.96	0.11	0.069	4	1.4	290.4	87.688	0.05	3	0.1	320	21
Sn	1.96	0.11	0.069	4	1.4	290.4	87.688	0.05	3	0.2	267	21
Sn	1.96	0.11	0.069	4	1.4	290.4	87.688	0.05	3	0.3	248	21
Sn	1.96	0.11	0.069	4	1.4	290.4	87.688	0.05	3	0.5	213	21
Sn	1.96	0.11	0.069	4	1.4	290.4	87.688	0.05	3	1	170	21

Sn	1.96	0.11	0.069	4	1.4	290.4	87.688	0.05	3	1.5	148	21
Sn	1.96	0.15	0.069	4	1.4	290.4	90.52	0.05	3	0.1	332	21
Sn	1.96	0.15	0.069	4	1.4	290.4	90.52	0.05	3	0.2	280	21
Sn	1.96	0.15	0.069	4	1.4	290.4	90.52	0.05	3	0.3	252	21
Sn	1.96	0.15	0.069	4	1.4	290.4	90.52	0.05	3	0.5	226	21
Sn	1.96	0.15	0.069	4	1.4	290.4	90.52	0.05	3	1	175	21
Sn	1.96	0.15	0.069	4	1.4	290.4	90.52	0.05	3	1.5	146	21
Cu	1.9	0.0544	0.077	1	1.12	157.3	80.74864	0.01	3	0.5	246	22
Cu	1.9	0.0544	0.077	1	1.12	157.3	80.74864	0.01	3	2	150	22
Cu	1.9	0.0544	0.077	1	1.12	157.3	80.74864	0.01	3	0.05	340	22
Cu	1.9	0.0544	0.077	1	1.12	157.3	80.74864	0.01	3	0.1	205	22
Cu	1.9	0.0544	0.077	1	1.12	157.3	80.74864	0.01	3	0.25	278	22
Cu	1.9	0.0544	0.077	1	1.12	157.3	80.74864	0.01	3	0.5	220	22
Cu	1.9	0.0544	0.077	1	1.12	157.3	80.74864	0.01	3	1	185	22
Cu	1.9	0.0233	0.077	1	1.12	157.3	80.26348	0.01	3	0.05	255	22
Cu	1.9	0.0233	0.077	1	1.12	157.3	80.26348	0.01	3	0.1	247	22
Cu	1.9	0.0233	0.077	1	1.12	157.3	80.26348	0.01	3	0.25	206	22
Cu	1.9	0.0233	0.077	1	1.12	157.3	80.26348	0.01	3	0.5	180	22
Cu	1.9	0.0233	0.077	1	1.12	157.3	80.26348	0.01	3	1	158	22
Cu	1.9	0.0233	0.077s	1	1.12	157.3	80.26348	0.01	3	2	143	22
Mn	1.55	0.031	0.067	2	1.19	519.7	80.117	1	2.5	0.03	185	23
Mn	1.55	0.031	0.067	2	1.19	519.7	80.117	1	2.5	0.15	160	23
Mn	1.55	0.031	0.067	2	1.19	519.7	80.117	1	2.5	0.5	145	23
Ni	1.91	0.05	0.069	2	1.1	239.7	80.44	1	3	0.335	138	24
Ni	1.91	0.05	0.069	2	1.1	239.7	80.44	1	3	6.7	72	24
Ni	1.91	0.05	0.069	2	1.1	239.7	80.44	1	3	0.0335	314	24
Ni	1.91	0.05	0.069	2	1.1	239.7	80.44	1	3	0.167	153	24
Ni	1.91	0.05	0.069	2	1.1	239.7	80.44	1	3	0.67	120	24
Ni	1.91	0.05	0.069	2	1.1	239.7	80.44	1	3	1.67	105	24
Zn	1.65	0.05	0.074	2	1.18	348.3	80.775	1	3.5	0.0335	190	25
Zn	1.65	0.05	0.074	2	1.18	348.3	80.775	1	3.5	0.167	168	25
Zn	1.65	0.05	0.074	2	1.18	348.3	80.775	1	3.5	0.835	110	25
Zn	1.65	0.05	0.074	2	1.18	348.3	80.775	1	3.5	1.67	75	25
Zn	1.65	0.05	0.074	2	1.18	348.3	80.775	1	3.5	3.35	45	25
Al	1.61	0.064	0.0535	3	1.26	1054	78.5624	1	3	0.335	175	26
Al	1.61	0.064	0.0535	3	1.26	1054	78.5624	1	3	1.67	118	26
Cr	1.66	0.05	0.0615	3	1.22	756.5	80.105	1.01	2.5	0.0335	218	27
Cr	1.66	0.05	0.0615	3	1.22	756.5	80.105	1.01	2.5	0.067	180	27
Cr	1.66	0.05	0.0615	3	1.22	756.5	80.105	1.01	2.5	0.167	175	27

Cr	1.66	0.05	0.0615	3	1.22	756.5	80.105	1.01	2.5	0.335	150	27
Cr	1.66	0.05	0.0615	3	1.22	756.5	80.105	1.01	2.5	1.67	110	27
Nb	1.6	0.065	0.069	5	1.47	379.9	82.825	1	3	0.042	168	28
Nb	1.6	0.065	0.069	5	1.47	379.9	82.825	1	3	0.056	160	28
Nb	1.6	0.065	0.069	5	1.47	379.9	82.825	1	3	0.084	140	28
Nb	1.6	0.065	0.069	5	1.47	379.9	82.825	1	3	1.67	125	28
Nb	1.6	0.065	0.069	5	1.47	379.9	82.825	1	3	0.335	110	28
Nb	1.6	0.065	0.069	5	1.47	379.9	82.825	1	3	0.67	88	28
Co	1.88	0.0121	0.061	3	1.11	606.6	80.0331	0.5	3	0.067	216	29
Co	1.88	0.0121	0.061	3	1.11	606.6	80.0331	0.5	3	0.335	185	29
Co	1.88	0.0121	0.061	3	1.11	606.6	80.0331	0.5	3	0.67	172	29
Co	1.88	0.0121	0.061	3	1.11	606.6	80.0331	0.5	3	1.67	149	29
Co	1.88	0.0121	0.061	3	1.11	606.6	80.0331	0.5	3	3.35	105	29
W	2.36	NAN	0.06	6	1.37	281	81.259	1	3	1	173	30
W	2.36	NAN	0.06	6	1.37	281	81.259	1	3	0.1	189	30
W	2.36	NAN	0.06	6	1.37	281	81.259	1	3	0.2	182	30
W	2.36	NAN	0.06	6	1.37	281	81.259	1	3	0.5	178	30
W	2.36	NAN	0.06	6	1.37	281	81.259	1	3	1	173	30
W	2.36	NAN	0.06	6	1.37	281	81.259	1	3	2	169	30
Sn	1.96	0.1	0.069	4	1.4	580.7	86.98	0.1	3	0.335	370	31
Sn	1.96	0.1	0.069	4	1.4	580.7	86.98	0.1	3	0.0335	440	31
Sn	1.96	0.1	0.069	4	1.4	580.7	86.98	0.1	3	1	340	31
Sn	1.96	0.1	0.069	4	1.4	580.7	86.98	0.1	3	1.67	325	31
Sn	1.96	0.1	0.069	4	1.4	580.7	86.98	0.1	3	3.35	290	31
Mn	1.55	0.279	0.067	2	1.19	519.7	81.853	0.01	3	0.4	275	32
Mn	1.55	0.279	0.067	2	1.19	519.7	81.853	0.01	3	0.8	205	32
Mn	1.55	0.279	0.067	2	1.19	519.7	81.853	0.01	3	1.6	165	32
Mn	1.55	0.279	0.067	2	1.19	519.7	81.853	0.01	3	3.2	147	32
Cu	1.9	0.15	0.073	2	1.12	157.9	82.255	1	3	0.167	243	33
Cu	1.9	0.15	0.073	2	1.12	157.9	82.255	1	3	0.335	235	33
Cu	1.9	0.15	0.073	2	1.12	157.9	82.255	1	3	0.67	223	33
Cu	1.9	0.15	0.073	2	1.12	157.9	82.255	1	3	1.67	190	33
Cu	1.9	0.15	0.073	2	1.12	157.9	82.255	1	3	3.35	175	33
Cu	1.9	0.15	0.073	2	1.12	157.9	82.255	1	3	5	160	33
Cu	1.9	0.15	0.073	2	1.12	157.9	82.255	1	3	6.7	152	33
Zr	1.33	0.01	0.072	4	1.54	547	80.333	1	3	0.0167	135	34
Zr	1.33	0.003	0.072	4	1.54	547	80.0299	1	3	0.0167	63	34
Zr	1.33	0.006	0.072	4	1.54	547	80.1598	1	3	0.0167	78	34
Zr	1.33	0.026	0.072	4	1.54	547	81.0258	1	3	0.0167	87	34

Sn	1.96	0.11	0.069	4	1.4	290.4	87.688	0.05	3	0.1	319	35
Sn	1.96	0.11	0.069	4	1.4	290.4	87.688	0.05	3	0.2	270	35
Sn	1.96	0.11	0.069	4	1.4	290.4	87.688	0.05	3	0.3	246	35
Sn	1.96	0.11	0.069	4	1.4	290.4	87.688	0.05	3	0.5	207	35
Sn	1.96	0.11	0.069	4	1.4	290.4	87.688	0.05	3	1	158	35
Sn	1.96	0.11	0.069	4	1.4	290.4	87.688	0.05	3	1.5	130	35
Cr	1.66	NAN	0.0615	3	1.22	756.5	80.105	1	3	0.084	110	14
Cr	1.66	NAN	0.0615	3	1.22	756.5	80.105	1	3	0.835	100	14
Cr	1.66	NAN	0.0615	3	1.22	756.5	80.105	1	3	0.167	140	14
Cr	1.66	NAN	0.0615	3	1.22	756.5	80.105	1	3	0.335	125	14
Mg	1.31	0.038	0.072	2	1.39	601.6	79.0032	1	3	0.0335	156	36
Mg	1.31	0.038	0.072	2	1.39	601.6	79.0032	1	3	0.084	148	36
Mg	1.31	0.038	0.072	2	1.39	601.6	79.0032	1	3	0.167	137	36
Mg	1.31	0.038	0.072	2	1.39	601.6	79.0032	1	3	0.501	112	36
Mg	1.31	0.038	0.072	2	1.39	601.6	79.0032	1	3	0.835	90	36
Mg	1.31	0.038	0.072	2	1.39	601.6	79.0032	1	3	1.67	73	36
Ti	1.62	0.04	0.067	3	1.36	1012	79.9	1	3	0.05	250	37
Ti	1.62	0.04	0.067	3	1.36	1012	79.9	1	3	0.1	205	37
Ti	1.62	0.04	0.067	3	1.36	1012	79.9	1	3	0.2	176	37
Ti	1.62	0.04	0.067	3	1.36	1012	79.9	1	3	0.5	151	37
Ti	1.62	0.04	0.067	3	1.36	1012	79.9	1	3	1	130	37
Ti	1.62	0.04	0.067	3	1.36	1012	79.9	1	3	2	96	37
Ti	1.62	0.04	0.067	3	1.36	1012	79.9	1	3	3	75	37
Zn	1.65	0.2	0.074	2	1.18	348.3	83.4	0.01	3	0.1	220	38
Zn	1.65	0.2	0.074	2	1.18	348.3	83.4	0.01	3	0.3	205	38
Zn	1.65	0.2	0.074	2	1.18	348.3	83.4	0.01	3	0.5	190	38
Zn	1.65	0.2	0.074	2	1.18	348.3	83.4	0.01	3	1	182	38
Zn	1.65	0.2	0.074	2	1.18	348.3	83.4	0.01	3	2	170	38
Zn	1.65	0.2	0.074	2	1.18	348.3	83.4	0.01	3	3	153	38
Nb	1.6	0.03	0.069	5	1.47	379.9	81.25	1	3	0.084	180	39
Nb	1.6	0.03	0.069	5	1.47	379.9	81.25	1	3	0.167	171	39
Nb	1.6	0.03	0.069	5	1.47	379.9	81.25	1	3	0.335	162	39
Nb	1.6	0.03	0.069	5	1.47	379.9	81.25	1	3	0.835	150	39
Nb	1.6	0.03	0.069	5	1.47	379.9	81.25	1	3	1.67	125	39
Nb	1.6	0.03	0.069	5	1.47	379.9	81.25	1	3	3.35	100	39
Nb	1.6	0.03	0.069	5	1.47	379.9	81.25	1	3	6.68	76	39
Nb	1.6	0.05	0.069	5	1.47	379.9	82.15	1	3	0.084	193	39
Nb	1.6	0.05	0.069	5	1.47	379.9	82.15	1	3	0.167	185	39
Nb	1.6	0.05	0.069	5	1.47	379.9	82.15	1	3	0.335	175	39

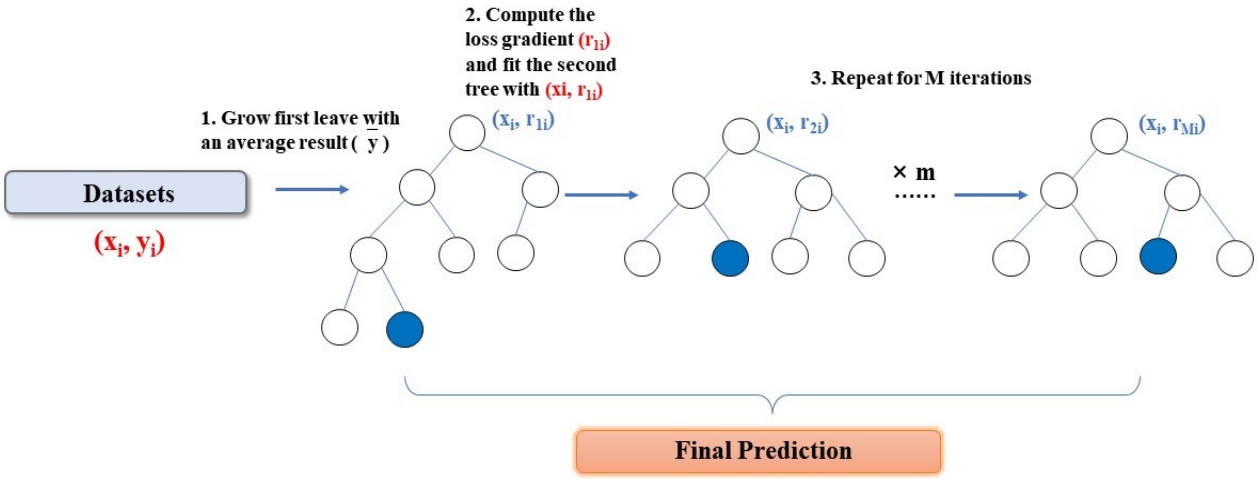
Nb	1.6	0.05	0.069	5	1.47	379.9	82.15	1	3	0.835	148	39
Nb	1.6	0.05	0.069	5	1.47	379.9	82.15	1	3	1.67	138	39
Nb	1.6	0.05	0.069	5	1.47	379.9	82.15	1	3	3.35	118	39
Nb	1.6	0.05	0.069	5	1.47	379.9	82.15	1	3	6.68	98	39
Nb	1.6	0.1	0.069	5	1.47	379.9	84.4	1	3	0.084	178	39
Nb	1.6	0.1	0.069	5	1.47	379.9	84.4	1	3	0.167	157	39
Nb	1.6	0.1	0.069	5	1.47	379.9	84.4	1	3	0.335	132	39
Nb	1.6	0.1	0.069	5	1.47	379.9	84.4	1	3	0.835	110	39
Nb	1.6	0.1	0.069	5	1.47	379.9	84.4	1	3	1.67	80	39
Nb	1.6	0.1	0.069	5	1.47	379.9	84.4	1	3	3.35	58	39
Nb	1.6	0.1	0.069	5	1.47	379.9	84.4	1	3	6.68	45	39
Ni	1.91	0.08	0.069	2	1.1	239.7	80.764	1	3	0.03	190	40
Ni	1.91	0.08	0.069	2	1.1	239.7	80.764	1	3	0.15	150	40
Ni	1.91	0.08	0.069	2	1.1	239.7	80.764	1	3	0.3	138	40
Ni	1.91	0.08	0.069	2	1.1	239.7	80.764	1	3	0.7	129	40
Ni	1.91	0.08	0.069	2	1.1	239.7	80.764	1	3	1.8	100	40

Supplementary Table S2. Names (units) and abbreviations of all the features.

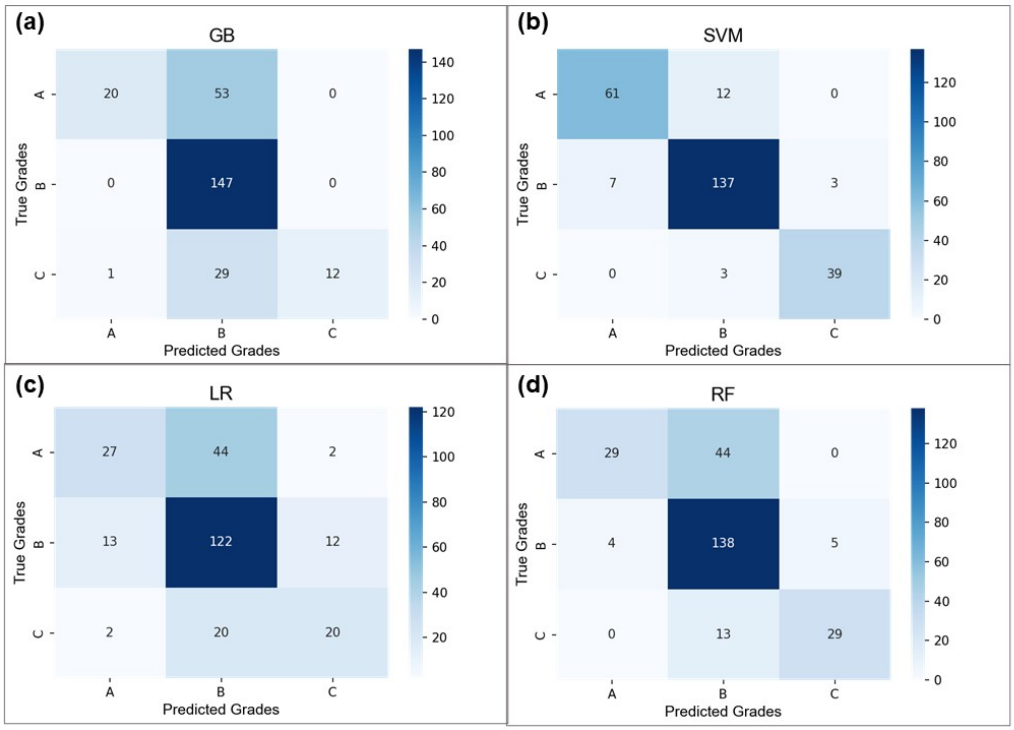
Features			
Dopant features		**Experiment features**	
Names (Units)	**Abbreviations**	**Names (Units)**	**Abbreviations**
Electronegativity of the doped elements	en	Current density (A/ g)	current
The atom ratio of dopant and Ti	ratio	Lowest potential during charging and discharging (V)	low
Dopant's ionic radius (nm)	radius	Highest potential during charging and discharging (V)	high
State of the dopant	state		
Material molecule mass	Mweight		
Molecule single bond covalent radius (nm)	rc		
Bond formation enthalpy of doped element and Oxygen (KJ)	feo		

Supplementary Table S3. Optimized hyperparameters of the models.

Hyperparameters of the models	
Random Forest Classifier (RF)	n_estimators=50, random_state=42, n_jobs = 5, max_depth = 3
Gradient Boosting Classifier (GB)	n_estimators=50, max_depth=3, random_state=42, learning_rate = 0.01
Support Vector Machine Classifier (SVM)	C = 27, gamma = 0.46, kernel='rbf'
Logistic Regression (LR)	C = 1.0, max_iter = 100, tol=0.0001
Support Vector Machine Regressor (SVM Regressor)	C = 27, gamma = 0.46
Random Forest Regressor (RF Regressor)	n_estimators=50, random_state=42, n_jobs = 5, max_depth = 3
Gradient Boosting Regressor (GB Regressor)	n_estimators=50, max_depth=3, random_state=42, learning_rate = 0.01
Miceforest	datasets=4, save_all_iterations=True, random_state=42, iterations=2, n_estimators=100



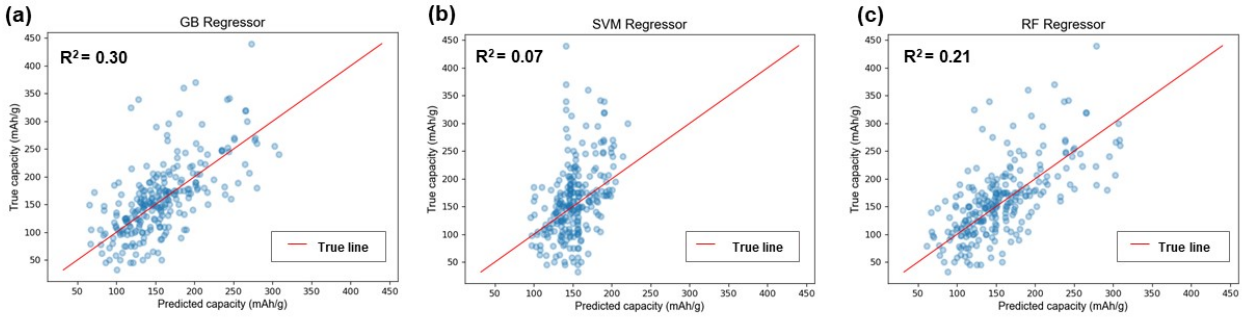
Supplementary Figure S1. Schematic illustration of GB classifier algorithm, where x_i denotes the value of the feature at the i^{th} sample, y_i is the capacity grade corresponding to x_i at the i^{th} sample.



Supplementary Figure S2. Confusion matrix generated from (a) GB model, (b) SVM model, (c) LR model, (d) RF model during cross-validation.

Supplementary Table S4. Comparison of Sensitivity (TPR), Specificity (TNR), Accuracy of 4 models (LR, SVM, RF, GB) results on cross-validation.

ML Models	Predictions on cross-validation		
	Sensitivity (TPR)	Specificity (TNR)	Accuracy
LR	0.64	0.82	0.64
SVM	0.90	0.95	0.90
RF	0.74	0.87	0.74
GB	0.69	0.84	0.69



Supplementary Figure S3. Plot scatter of true capacity and predicted capacity of (a) GB Regressor, (b) SVM Regressor, (c) RF Regressor, where R^2, given from equation S1, was calculated to evaluate the models (where $\hat{y}^{(i)}$ is the predicted value, $y^{(i)}$ is the true value, $\bar{y}$ is the average of the true values.)

$$R^2 = 1 - \frac{\sum_i (\hat{y}^{(i)} - y^{(i)})^2}{\sum_i (\bar{y} - y^{(i)})^2} \quad \text{(S1)}$$

Supplementary Table S5. Comparison of Sensitivity (TPR), Specificity (TNR), Accuracy of GB

model's results on test set using the top 8 features and the last 8 features in Figure 5 respectively.

	Prediction on test set		
	Sensitivity (TPR)	Specificity (TNR)	Accuracy
Using the top 8 features	0.74	0.87	0.74
Using the last 8 features	0.68	0.80	0.68

References

1. Q. Cheng, S. Tang, C. Liu, Q. Lan, J. Zhao, J. Liang, J. Yan, Z. Liu and Y.-C. Cao, Preparation and electrochemical performance of $Li_{4-x}Mg_xTi_5O_{12}$ as anode materials for lithium-ion battery, *J. Alloys Compd.*, 2017, **722**, 229-234.
2. C. Yu, Y. Bai, D. Yan, X. Li and W. Zhang, Improved electrochemical properties of Sn-doped TiO_2 nanotube as an anode material for lithium ion battery, *J. Solid State Electrochem.*, 2014, **18**, 1933-1940.
3. M. Lübke, J. Shin, P. Marchand, D. Brett, P. Shearing, Z. Liu and J. A. Darr, Highly pseudocapacitive Nb-doped TiO_2 high power anodes for lithium-ion batteries, *J. Mater. Chem. A.*, 2015, **3**, 22908-22914.
4. Y. Li, S. Zhu, A. Inoue, Y. Liang, C. Chang, S. Luo and Z. Cui, Preparation of nanoporous Sn-doped TiO_2 anode material for lithium-ion batteries by a simple dealloying method, *Ionics*, 2020, **26**, 4363-4372.
5. Y. Lai, W. Liu, J. Fang, F. Qin, M. Wang, F. Yu and K. Zhang, Fe-doped anatase TiO_2/carbon composite as an anode with superior reversible capacity for lithium storage, *RSC Adv.*, 2015, **5**, 93676-93683.
6. S. Huang, L. Zhang, X. Lu, L. Liu, L. Liu, X. Sun, Y. Yin, S. Oswald, Z. Zou, F. Ding and O. G.

Schmidt, Tunable Pseudocapacitance in 3D $TiO_{(2-\delta)}$ Nanomembranes Enabling Superior Lithium Storage Performance, *ACS Nano*, 2017, **11**, 821-830.

7. A. J. Gardecka, M. Lübke, C. F. Armer, D. Ning, M. V. Reddy, A. S. Williams, A. Lowe, Z. Liu, I. P. Parkin and J. A. Darr, Nb-doped rutile titanium dioxide nanorods for lithium-ion batteries, *Solid State Sci.*, 2018, **83**, 115-121.
8. D. Kang, J. Li and Y. Zhang, Effect of Ni Doping Content on Phase Transition and Electrochemical Performance of TiO(2) Nanofibers Prepared by Electrospinning Applied for Lithium-Ion Battery Anodes, *Materials*, 2020, **13**, 1302.
9. D. P. Opra, S. V. Gnedenkov, S. L. Sinebryukhov, A. B. Podgorbunsky, A. A. Sokolov, A. Y. Ustinov, V. G. Kuryavyi, V. Y. Mayorov and V. V. Zheleznov, Doping of titania with manganese for improving cycling and rate performances in lithium-ion batteries, *Chem. Phys.*, 2020, **538**, 110864.
10. Y. Wang, M. Xu, Z. Peng and G. Zheng, Direct growth of mesoporous Sn-doped TiO_2 thin films on conducting substrates for lithium-ion battery anodes, *J. Mater. Chem. A.*, 2013, **1**, 13222-13226.
11. C. T. Kacica and P. Biswas, Improved conductivity and ionic mobility in nanostructured thin films via aliovalent doping for ultra-high rate energy storage, *Nanoscale Adv.*, 2020, **2**, 2160-2169.
12. W. Zhang, Y. Gong, N. P. Mellott, D. Liu and J. Li, Synthesis of nickel doped anatase titanate as high performance anode materials for lithium ion batteries, *J. Power Sources*, 2015, **276**, 39-45.
13. Y. Zhang, Y. Meng, K. Zhu, H. Qiu, Y. Ju, Y. Gao, F. Du, B. Zou, G. Chen and Y. Wei, Copper-Doped Titanium Dioxide Bronze Nanowires with Superior High Rate Capability for

Lithium Ion Batteries, *ACS Appl. Mater. Interfaces*, 2016, **8 12**, 7957-7965.

14. H. Xu, M. Zeng, J. Li and F. Li, Cr-Doped TiO_2 Core–Shell Nanospheres with Enhanced Photocatalytic Activity and Lithium Storage Capacity, *Nano*, 2016, **11**, 1650006.
15. A. A. Kashale, A. S. Rasal, G. P. Kamble, V. H. Ingole, P. K. Dwivedi, S. J. Rajoba, L. D. Jadhav, Y.-C. Ling, J.-Y. Chang and A. V. Ghule, Biosynthesized Co-doped TiO_2 nanoparticles based anode for lithium-ion battery application and investigating the influence of dopant concentrations on its performance, *Compos. B. Eng.*, 2019, **167**, 44-50.
16. D. Yan, C. Yu, Y. Bai, W. Zhang, T. Chen, B. Hu, Z. Sun and L. Pan, Sn-doped TiO_2 nanotubes as superior anode materials for sodium ion batteries, *Chem. Comm.*, 2015, **51**, 8261-8264.
17. Y. Liu, X. Pan, W. Chen and X. Zhao, Titanate-derived Nb-doped TiO2 nanoparticles displaying improved lithium storage performance, *Dalton Trans.*, 2022, **51**, 2506-2511.
18. Y. Tanaka, H. Usui, Y. Domi, M. Ohtani, K. Kobiro and H. Sakaguchi, Mesoporous Spherical Aggregates Consisted of Nb-Doped Anatase TiO_2 Nanoparticles for Li and Na Storage Materials, *ACS Appl. Energy Mater.*, 2019, **2**, 636-643.
19. C. Cavallo, G. Calcagno, R. P. de Carvalho, M. Sadd, B. Gonano, C. M. Araujo, A. E. C. Palmqvist and A. Matic, Effect of the Niobium Doping Concentration on the Charge Storage Mechanism of Mesoporous Anatase Beads as an Anode for High-Rate Li-Ion Batteries, *ACS Appl. Energy Mater.*, 2021, **4**, 215-225.
20. Y. Fan, X. Chen, K. Zhang, J. Rong and X. Yu, A coordinated regulation strategy to improve electronic conductivity and Li-ion transport for TiO_2 lithium battery anode materials, *J. Alloys Compd.*, 2021, **860**, 158282.
21. M. Lübke, I. Johnson, N. M. Makwana, D. Brett, P. Shearing, Z. Liu and J. A. Darr, High power

TiO2 and high capacity Sn-doped TiO_2 nanomaterial anodes for lithium-ion batteries, *J. Power Sources*, 2015, **294**, 94-102.

22. A. A. Kashale, P. K. Dwivedi, B. R. Sathe, M. V. Shelke, J. Y. Chang and A. V. Ghule, Biomass-Mediated Synthesis of Cu-Doped TiO(2) Nanoparticles for Improved-Performance Lithium-Ion Batteries, *ACS Omega*, 2018, **3**, 13676-13684.
23. W. Zhang, W. Zhou, J. H. Wright, Y. N. Kim, D. Liu and X. Xiao, Mn-Doped TiO_2 Nanosheet-Based Spheres as Anode Materials for Lithium-Ion Batteries with High Performance at Elevated Temperatures, *ACS Appl. Mater. Interfaces*, 2014, **6**, 7292-7300.
24. R. Ata ur, G. Ali, S. M. Abbas, M. Iftikhar, M. Zahid, S. Yaseen, S. Saleem, S. Haider, M. Arshad and A. Badshah, Axial expansion of Ni-doped TiO_2 nanorods grown on carbon nanotubes for favourable lithium-ion intercalation, *Chem. Eng. J.*, 2019, **375**, 122021.
25. Z. Ali, S. N. Cha, J. I. Sohn, I. Shakir, C. Yan, J. M. Kim and D. J. Kang, Design and evaluation of novel Zn doped mesoporous TiO_2 based anode material for advanced lithium ion batteries, *J. Mater. Chem.*, 2012, **22**, 17625-17629.
26. C. Zhang, Y. Qi, S. Liu, Y. Men and F. Cui, Novel mesoporous Al-doped TiO_2 with improved lithium storage performance, *Mater. Chem. Phys.*, 2019, **237**, 121822.
27. Z. Bi, M. P. Paranthaman, B. Guo, R. R. Unocic, H. M. Meyer Iii, C. A. Bridges, X.-G. Sun and S. Dai, High performance Cr, N-codoped mesoporous TiO_2 microspheres for lithium-ion batteries, *J. Mater. Chem. A*, 2014, **2**, 1818-1824.
28. Y. Wang, B. M. Smarsly and I. Djerdj, Niobium Doped TiO_2 with Mesoporosity and Its Application for Lithium Insertion, *Chem. Mater.*, 2010, **22**, 6624-6631.
29. C. Zhang, D. Shao, J. Yu, L. Zhang, X. Huang, D. Xu and X. Yu, Synthesis and electrochemical

performance of cubic Co-doped $Li_4Ti_5O_{12}$ anode material for high-performance lithium-ion batteries, *J. Electroanal. Chem.*, 2016, **776**, 188-192.

30. Z. Pu, Q. Lan, Y. Li, S. Liu, D. Yu and X.-J. Lv, Preparation of W-doped hierarchical porous $Li_4Ti_5O_{12}$/brookite nanocomposites for high rate lithium ion batteries at − 20 °C, *J. Power Sources*, 2019, **437**, 226890.
31. T.-Y. Chen, Y.-T. Liu, P.-C. Wu, C.-W. Hu, P.-W. Yang, L.-C. Hsu, C.-H. Lee and C.-C. Chang, Lithiation-induced crystal restructuring of hydrothermally prepared Sn/TiO_2 nanocrystallite with substantially enhanced capacity and cycling performance for lithium-ion battery, *RSC Adv.*, 2016, **6**, 48620-48629.
32. J. Wang, G. Yang, L. Wang, S. Wang, W. Yan and S. Ding, In-situ fabrication of transition-metal-doped TiO_2 nanofiber/nanosheet structure for high-performance Li storage, *J. Alloys Compd.*, 2019, **787**, 1110-1119.
33. Y. Zhang, Y. Meng, K. Zhu, H. Qiu, Y. Ju, Y. Gao, F. Du, B. Zou, G. Chen and Y. Wei, Copper-Doped Titanium Dioxide Bronze Nanowires with Superior High Rate Capability for Lithium Ion Batteries, *ACS Appl. Mater. Interfaces*, 2016, **8 12**, 7957-7965.
34. D. P. Opra, S. V. Gnedenkov, S. L. Sinebryukhov, E. I. Voit, A. A. Sokolov, E. B. Modin, A. B. Podgorbunsky, Y. V. Sushkov and V. V. Zheleznov, Characterization and Electrochemical Properties of Nanostructured Zr-Doped Anatase TiO_2 Tubes Synthesized by Sol–Gel Template Route, *J. Mater. Sci. Technol.*, 2017, **33**, 527-534.
35. M. Lübke, I. Johnson, N. M. Makwana, D. Brett, P. Shearing, Z. Liu and J. A. Darr, High power TiO2 and high capacity Sn-doped TiO_2 nanomaterial anodes for lithium-ion batteries, *J. Power Sources*, 2015, **294**, 94-102.

36. X. Bai, W. Li, A. Wei, X. Li, L. Zhang and Z. Liu, Preparation and electrochemical properties of Mg^{2+} and F^{-} co-doped $Li_4Ti_5O_{12}$ anode material for use in the lithium-ion batteries, *Electrochim. Acta*, 2016, **222**, 1045-1055.

37. Y. Ren, J. Li and J. Yu, Enhanced electrochemical performance of TiO_2 by Ti^{3+} doping using a facile solvothermal method as anode materials for lithium-ion batteries, *Electrochim. Acta*, 2014, **138**, 41-47.

38. H. Li, Z. Li, Y. Cui, C. Ma and Z. Tang, Long-cycled $Li_2ZnTi_3O_8/TiO_2$ composite anode material synthesized via a one-pot co-precipitation method for lithium ion batteries, *New J. Chem.*, 2017, **41**, 975-981.

39. T. Lan, W. Zhang, N.-L. Wu and M. Wei, Nb-Doped Rutile TiO_2 Mesocrystals with Enhanced Lithium Storage Properties for Lithium Ion Battery, *Chem. Eur. J.*, 2017, **23**, 5059-5065.

40. D. P. Opra, S. V. Gnedenkov, S. L. Sinebryukhov, A. V. Gerasimenko, A. M. Ziatdinov, A. A. Sokolov, A. B. Podgorbunsky, A. Y. Ustinov, V. G. Kuryavyi, V. Y. Mayorov, I. A. Tkachenko and V. I. Sergienko, Enhancing Lithium and Sodium Storage Properties of TiO_2(B) Nanobelts by Doping with Nickel and Zinc. *Nanomaterials* 2021, **11**, 1703.