# Contents lists available at ScienceDirect

# Journal of Power Sources

journal homepage: www.elsevier.com/locate/jpowsour

# Potential of porous nodal-line semi-metallic carbon for sodium-ion battery anode

# Yupeng Shen<sup>a</sup>, Qian Wang<sup>a,\*</sup>, Y. Kawazoe<sup>b,c,d</sup>, Puru Jena<sup>e</sup>

<sup>a</sup> Center for Applied Physics and Technology, Department of Materials Science and Engineering, HEDPS, BKL-MEMD, College of Engineering, Peking University, Beijing, 100871, China

<sup>b</sup> New Industry Creation Hatchery Center, Tohoku University, Sendai, 980-8577, Japan

<sup>c</sup> Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, 603203, India

<sup>d</sup> Suranaree University of Technology, Nakhon Ratchasima, 30000, Thailand

<sup>e</sup> Department of Physics, Virginia Commonwealth University, Richmond, VA, 23284, USA

### HIGHLIGHTS

• Small volume change.

Intrinsic high electric conductivity.High capacity and low energy barrier.

#### G R A P H I C A L A B S T R A C T



# ARTICLE INFO

Keywords: Carbon Anode Nodal-line semi-metallic Sodium-ion battery DFT

# ABSTRACT

As an alternative to lithium-ion batteries (LIBs), sodium-ion batteries (SIBs) have attracted much attention because sodium is abundant, cost-effective, and environmentally benign. However, due to the larger size of Naion compared to the Li-ion, graphite does not work well as an anode for SIBs, as it does for LIBs. Here, based on first-principles calculations, we show that the recently proposed topological semi-metallic carbon, HZGM-42, has great potential as an anode material for SIBs. With a large capacity of 318.5 mAhg<sup>-1</sup>, low diffusion barrier of 0.08–0.21 eV, low average open-circuit voltage of 0.43 V, and a small volume expansion of 1.85%, the all-carbon topological quantum HZGM-42 has high energy density, good rate capability, and excellent cycling stability and can serve as a universal anode material for both LIBs and SIBs.

#### 1. Introduction

Due to the excellent performance and successful commercialization, LIBs are widely used in various technologies such as mobile devices, electric vehicles, and medical equipment [1-3]. However, with smart

power grids receiving increasing attention, the demand for large-scale energy storage is growing rapidly [4,5]. Due to the limited lithium resources in continental crust with a concentration of 0.0018% [6], LIBs will not be able to meet the demand for large-scale energy storage devices [7,8]. Therefore, it is crucial to find an alternative to lithium that is

https://doi.org/10.1016/j.jpowsour.2020.228746

Received 13 June 2020; Received in revised form 15 July 2020; Accepted 3 August 2020 Available online 29 August 2020 0378-7753/© 2020 Published by Elsevier B.V.



Perspective



<sup>\*</sup> Corresponding author. E-mail address: qianwang2@pku.edu.cn (Q. Wang).

cheap and abundant. SIBs are considered to be suitable substitutes for LIBs because of the high abundance of sodium in continental crust with a concentration of 2.36% [6] as well as its environment-friendly nature [9] and low cost [10,11]. However, due to the large ionic radius of Na (1.02 Å for Na vs 0.76 Å for Li) as well as their different electrochemical potentials [12,13], the anode materials that perform well in LIBs usually show poor performance in SIBs [14,15]. For example, graphite, which is commercially used in LIBs with great success, has a limited capacity of only 35 mAhg<sup>-1</sup> in SIBs [16,17]. Therefore, it is highly desirable to find suitable anode materials for SIBs.

Much effort has been devoted to developing anode materials for SIBs, and many such materials have been proposed. However, these materials are usually accompanied by some disadvantages that affect their performance. For instance, phosphorus and phosphide anodes do possess large capacities, but they are plagued by large volume expansion [18–20]. In addition, flammable and toxic PH<sub>3</sub> is produced during the fabrication process, causing safety issues [21,22]. Metal oxide anodes such as Fe<sub>2</sub>O<sub>3</sub> [23] and TiO<sub>2</sub> [24] suffer from poor electrical conductivity and toxicity (such as PbO [25]). Similarly, metal sulfide and selenide anodes show relatively low conductivity and large volume expansion [26–28].

Compared to the above materials, carbon anode for SIBs is of particular interest because of its rich resource, low cost, various morphologies, and environmental compatibility [29-31]. The recently synthesized porous carbon materials used as the anodes for SIBs are usually amorphous [32,33], where the disordered holes and defects affect the transport of sodium ion and reduce electronic conductivity [34]. Hence, it is important to find carbon-based anode materials having regular channels and intrinsic high electrical conductivity. Recently, a 3D nodal-line semi-metallic porous carbon, HZGM-42, was proposed [35] as a promising anode candidate for LIBs with a high theoretical specific capacity of 637.71 mAhg<sup>-1</sup>, a low energy barrier of 0.02 eV for Li ion diffusion along the one-dimensional channels, and a small volume change of 2.4% during charging and discharging operation. Since the pore size in HZGM-42 is larger than the interlayer distance in graphite, and its intrinsic good electrical conductivity is protected by the topology, we expected this structure to have significant advantage over disordered carbon, metal oxide, metal sulfide and selenide anodes [23-28] that exhibit poor electrical conductivity. Our systematic first-principles study confirms this expectation.

#### 2. Computational methods

First-principles calculations based on density functional theory (DFT) are performed using the projector augmented wave (PAW) method [36] as implemented in the Vienna Ab initio Simulation Package (VASP) [37]. The Perdew-Burke-Ernzerhof (PBE) functional within the generalized gradient approximation (GGA) [38] is adopted to treat the electron exchange-correlation interactions. The energy cutoff is set to 520 eV for the wave functions. For structure optimization, the convergence thresholds of total energy and force are set as  $10^{-6}\ \text{eV}$  and  $10^{-4}$ eVÅ  $^{-1},$  respectively. The Brillouin zone is represented by a 4  $\times$  4  $\times$  21 kpoints mesh within the Monkhorst-Pack scheme [39]. The nudged elastic band (NEB) method [40,41] is used to calculate the diffusion barriers of sodium ions. To obtain the lowest energy structure for each Na adsorption concentration, we use the pymatgen package [42] to find all possible structures with unconstrained symmetry for every intermediate concentration, and then calculate the energies with both electrostatic Ewald energy method and DFT, which has been adopted in many previous studies [43-45].

## 3. Results and discussion

HZGM-42 is a 3D structure composed of zigzag graphene nano ribbons connected by the four-fold coordinated carbon chains as linkers. The top view of the unit cell and the side view of the  $1 \times 1 \times 4$  supercell

are shown in Fig. 1a and b, respectively. HZGM-42 has hexagonal symmetry with 42 carbon atoms in its unit cell. The lattice parameters of the fully relaxed structure are a = b = 16.80 Å and c = 2.46 Å, which are consistent with the previous results [35].

We first study the adsorption of a single Na atom on HZGM-42. To avoid interaction between the Na atoms, we adopt a  $1 \times 1 \times 4$  supercell. Five possible nonequivalent initial adsorption sites are considered according to the geometric symmetry of HZGM-42, as shown in Fig. 1a and b. For convenience, the Na atom adsorbed at position x (x = 1, 2, 3, 4, 5) is labeled Na<sub>x</sub>. Na<sub>1</sub>, Na<sub>2</sub> and Na<sub>3</sub> reside in the small pore, while Na<sub>4</sub> and Na<sub>5</sub> are in the large pore of this structure. Specifically, Na<sub>1</sub> is located at the corner of the triangle consisting of graphene nanoribbons, Na<sub>2</sub> is at the bridge site of the side chain, and Na<sub>3</sub> is at the hollow site of the triangle. Na<sub>4</sub> is located near the bridge site of the side chain while Na<sub>5</sub> is near the corner. To check the binding strength of Na atoms on these adsorption sites, we calculate the adsorption energy ( $E_a$ ) using the following formula:

$$E_a = E_2 - E_1 - E_{Na}, (1)$$

Here,  $E_2(E_1)$  is the total energy of system with (without) the adsorbed Na atom, and  $E_{Na}$  is the energy of one Na atom in its bulk phase. After structure relaxation, Na<sub>2</sub> and Na<sub>3</sub> move to position 1, and Na<sub>4</sub> moves to position 5. The adsorption energies for Na<sub>1</sub> and Na<sub>5</sub> are -1.22 and -0.78 eV, respectively, indicating that Na can be easily absorbed on HZGM-42. Bader charge analysis [46] shows that the charges on Na<sub>1</sub> and Na<sub>5</sub> are 0.87 and 0.88 electrons, respectively, indicating that most of the 3s electrons of Na atom are transferred to the substrate, leading to good binding between the Na-ions and the carbon substrate. Meanwhile, the strong Coulomb repulsion between Na ions will prevent them from clustering, thus ensuring a good performance of the anode.

Next, we calculate the energy barrier for Na-ion diffusion in HZGM-42 to determine the rate capability. According to the structural symmetry and Na adsorption sites, we select two possible diffusion pathways, marked as path 1 and path 2 in Fig. 2a. The diffusion energy barrier profiles for path 1 and path 2 are calculated and plotted in Fig. 2b and c, respectively. The corresponding diffusion barriers are 0.08 and 0.07 eV, respectively, which are much lower than that in many other anode materials for SIBs, such as T-C<sub>24</sub> (0.13 eV) [34], 17-MoS<sub>2</sub> (0.28 eV) [47], 2*H*-MoS<sub>2</sub> (0.68 eV) [47] and Si<sub>24</sub> (0.68 eV) [48]. For the convenience of comparison, these results are summarized in Table 1. The low diffusion barrier indicates that Na-ions can migrate easily in the structure. Due to the intrinsic high electrical conductivity protected by the topology of this structure, HZGM-42 possesses good rate capability.

We explore the maximum capacity of HZGM-42 by gradually increasing the amount of adsorbed Na, and find that the maximum adsorption corresponds to NaC<sub>7</sub>, leading to a theoretical maximum specific capacity of 318.5 mAhg<sup>-1</sup> (see Fig. 1c and d). This capacity is much larger than that of many other reported SIB anodes, including Si<sub>24</sub> (159 mAhg<sup>-1</sup>) [48] 1*T*-MoS<sub>2</sub> (86 mAhg<sup>-1</sup>) [47], 2*H*-MoS<sub>2</sub> (146 mAhg<sup>-1</sup>) [47], ISN (159.5 mAhg<sup>-1</sup>) [49] and T-C<sub>24</sub> (232.6 mAhg<sup>-1</sup>) [34] (see Table 1), indicating that HZGM-42 is a promising anode material for SIBs with high capacity.

To further examine the migration of Na-ions, we consider the system with maximum Na concentration, namely, NaC<sub>7</sub>. We remove one Na-ion from the fully adsorbed structure and study the diffusion of the resulting vacancy. As shown in Fig. 3a, two paths are selected according to the symmetry of the structure. The corresponding energy barrier plots are shown in Fig. 3b and c. One can see that although the barriers of path 1 (0.21 eV) and path 2 (0.10 eV) are larger than those of single Na-ion diffusion, these values are still quite small. The low diffusion barriers of vacancy indicate that Na-ions can migrate smoothly even at a high concentration, leading to a good rate capability for HZGM-42.

To study the battery performance, we calculate the average circuit voltage by using the following half-cell reaction model:



**Fig. 1.** (a) Top and (b) side views of the geometric structure of a  $1 \times 1 \times 4$  supercell of HZGM-42 with five possible adsorption sites. The magnified images for these absorption positions are also plotted in (a). (c) Top and (d) side views of the stable adsorption structure with the maximum Na concentration (NaC<sub>7</sub>).



Fig. 2. (a) Two possible diffusion pathways of Na-ions in HZGM-42. (b) and (c) present the corresponding energy barrier plots for diffusion along path 1 and path 2, respectively.

#### Table 1

Diffusion barrier (in eV), specific capacity (in  $mAhg^{-1}$ ), open-circuit voltage (in V) and percentage volume change (%) of HZGM-42 and some other reported anode materials for SIBs.

Materials	Diffusion barrier	Specific capacity	Open-circuit voltage	Volume change
HZGM- 42	0.08	318.5	0.43	1.85
Si <sup>48</sup> Si <sup>24</sup>	0.68	159	0.30	2.30
1T-MoS <sub>2</sub> <sup>47</sup>	0.28	86	1.25	27.5
2H-	0.68	146	0.75	27.1
MoS <sub>2</sub> <sup>47</sup>				
ISN <sup>49</sup>	0.005	159.5	1.35	2.80
T-C <sup>34</sup>	0.13	232.6	0.54	0.94

$$(x_2 - x_1)Na^+ + (x_2 - x_1)e^- + Na_{x1} - HZGM - 42 \leftrightarrow Na_{x2} - HZGM - 42$$
(2)

Ignoring the effect of volume, pressure and entropy, we calculate the average voltage *V* in the concentration range  $x_1 < x < x_2$  using the following equation:

$$V \approx \frac{E_{Na_{x1} - HZGM - 42} - E_{Na_{x2} - HZGM - 42} + (x_2 - x_1)E_{Na}}{x_2 - x_1}$$
(3)

Here,  $E_{Na_{x1}-HZGM-42}$  and  $E_{Na_{x2}-HZGM-42}$  are the total energies of Na absorbed structures with concentrations of  $x_1$  and  $x_2$ , respectively. To obtain the total energies for the five different intermediate concentrations (Na<sub>x</sub>C<sub>7</sub>: x = 0.167, 0.333, 0.5, 0.667, and 0.833), the optimal structures for each of these concentrations need to be determined. We



Fig. 3. (a) Two possible diffusion pathways of the vacancy in HZGM-42. The red spheres in (a) represent the vacancy. The corresponding energy barrier plots for diffusion path 1 (b) and path 2 (c). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

chose twenty configurations for each adsorption concentration and find the configuration with lowest energy as the optimal structure. The schematics of optimal structures for the five intermediate concentrations are plotted in Fig. 4, where Na-ions tend to be uniformly dispersed in the structures to reduce the Coulomb repulsion, thus leading to lower total energies. We note that the structures of HZGM-42 still remain nearly intact when Na atoms are adsorbed at different concentrations, suggesting that HZGM-42 can work stably during the charging and discharging process.

Based on the optimal structures, the variations of the binding energies of Na-ions and the voltage with Na concentration are plotted in

Fig. 5a and b, respectively. As the concentration increases, the absolute value of the binding energy gradually decreases because of the repulsive interactions between the Na-ions. In the whole adsorption process, the voltage curve can be divided into two voltage plateaus, separated by the concentration of 0.167, at which the voltage drops from 1.04 to 0.47 V. After that, the voltage slowly decreases from 0.47 to 0.22 V with increasing concentration. The voltage value remains positive throughout the whole concentration range, implying that the half-cell reaction can proceed spontaneously until it reaches the final state NaC<sub>7</sub>, resulting in a fully reversible capacity of 318.5 mAhg<sup>-1</sup>. In order to better characterize the overall voltage, we calculate the average open-



Fig. 4. Top and side views of the most stable configuration of  $Na_xC_7$  with (a) x = 0.167, (b) x = 0.333, (c) x = 0.5, (d) x = 0.667, and (e) x = 0.833.



**Fig. 5.** (a) Variation of the binding energy and (b) the voltage with Na concentration for  $Na_xC_7$ . The lowest energy for each concentration is highlighted in red. (b) Voltage vs concentration plot for HZGM-42. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

circuit voltage by numerically averaging the whole voltage profile. The average open-circuit voltage of HZGM-42 is calculated to be 0.43 V, which is lower than the value of 1T-MoS<sub>2</sub> (1.25 V) [47], 2*H*-MoS<sub>2</sub> (0.75 V) [47], ISN (1.35 V) [49] and T-C<sub>24</sub> (0.54 V) [34]. The low average voltage is favorable for a high voltage fully assembled battery when the anode is connected with the cathode.

Among the parameters measuring the anode performance, cycling stability is also important, as it reflects the long-term performance of an anode. If the structure of an anode material undergoes serious deformation after adsorption, the properties of the anode, such as capacity, would rapidly degrade after a few cycles [50,51]. To evaluate the cyclic stability of HZGM-42, we calculate the percentage of volume change after full Na adsorption, which is found to be 1.85%. This change is much smaller than the reported values for other systems: 10.6% for hard carbon [52], 27.5% for 1*T*-MoS<sub>2</sub> [47], and 27.1% for 2*H*-MoS<sub>2</sub> [47], and is even smaller than that for Si<sub>24</sub> (2.3%) [48] and ISN (2.8%) [49]. These results indicate that HZGM-42 may possess excellent cycling stability.

#### 4. Conclusions

Different from previous studies of topological quantum materials either for LIBs [35,53-55] or SIBs [34,49], we have found, for the first time, that the recently proposed porous nodal-line semi-metallic carbon HZGM-42 is a good candidate for SIBs anode as it is for LIBs. Based on first-principles calculations, we have demonstrated that HZGM-42 has the following attractive characteristics: (1) a higher capacity of 318.5  $mAhg^{-1}$ , as compared to many other SIB anode materials; (2) low diffusion barrier of 0.08-0.21 eV, indicating good rate capability; (3) low average voltage of 0.43 V, showing voltage advantage when constituting a full battery; and (4) low volume expansion of 1.85%. Considering that HZGM-42 as an anode material for LIBs has a high theoretical specific capacity of 637.71 mAhg<sup>-1</sup>, a low energy barrier of 0.02 eV, and a small volume change of 2.4% [35], we conclude that it could serve as a universal promising all-carbon quantum topological anode material, going beyond the existing studies. We hope that our study will stimulate further experimental effort in this direction.

# CRediT authorship contribution statement

Yupeng Shen: Conceptualization, Writing - original draft, Methodology, Software, Formal analysis, Investigation, Data curation, Visualization. Qian Wang: Conceptualization, Funding acquisition, Project administration, Software, Writing - review & editing, Validation, Resources, Supervision. Y. Kawazoe: Validation, Resources, Writing - review & editing, Funding acquisition. Puru Jena: Validation, Resources, Writing - review & editing, Funding acquisition.

#### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

#### Acknowledgments

This work is partially supported by grants from the National Natural Science Foundation of China (Grants No. NSFC-11974028, and NSFC-21773004) and the National Key Research and Development Program of China (Grant No.2017YFA0205003). Y. K. acknowledges the financial support from JSPS Kakenhi Grant no. 17H03384 and HPCI Project hp190111. P. J. acknowledges support by the U.S DOE, Office of Basic Energy Sciences, Division of Material Sciences and Engineering under Award No. DE-FG02-96ER45579. The authors thank the crew of High Performance Computing Platform of Peking University, and the Center for Computational Materials Science, the Institute for Materials Research, Tohoku University (Japan), for their continuous support of the MASAMUNE-IMR supercomputing facility.

# References

- J.-M. Tarascon, M. Armand, Issues and challenges facing rechargeable lithium batteries, in: Materials for Sustainable Energy: a Collection of Peer-Reviewed Research and Review Articles from Nature Publishing Group, World Scientific, 2011, pp. 171–179.
- [2] Z. Fang, J. Wang, H. Wu, Q. Li, S. Fan, J. Wang, J. Power Sources 454 (2020) 227932.
- [3] Z. Hu, Q. Liu, S.L. Chou, S.X. Dou, Adv. Mater. 29 (2017) 1700606.
- [4] J.Y. Hwang, S.T. Myung, Y.K. Sun, Adv. Funct. Mater. 28 (2018) 1802938.
  [5] Y. Shen, J. Liu, X. Li, Q. Wang, ACS Appl. Mater. Interfaces 11 (2019)
- 35661–35666.
- [6] K.H. Wedepohl, Geochem. Cosmochim. Acta 59 (1995) 1217-1232.
- [7] T. Liu, Y. Zhang, Z. Jiang, X. Zeng, J. Ji, Z. Li, X. Gao, M. Sun, Z. Lin, M. Ling, Energy Environ. Sci. 12 (2019) 1512–1533.
- [8] L. Ran, I. Gentle, T. Lin, B. Luo, N. Mo, M. Rana, M. Li, L. Wang, R. Knibbe, J. Power Sources 461 (2020) 228116.
- [9] S.W. Kim, D.H. Seo, X. Ma, G. Ceder, K. Kang, Adv. Energy Mater. 2 (2012) 710–721.
- [10] Q. Jin, W. Li, K. Wang, P. Feng, H. Li, T. Gu, M. Zhou, W. Wang, S. Cheng, K. Jiang, J. Mater. Chem. A 7 (2019) 10239–10245.
- [11] C. Luo, J.J. Shea, J. Huang, J. Power Sources 453 (2020) 227904.
- [12] B. Xiao, T. Rojo, X. Li, ChemSusChem 12 (2019) 133–144.
- [13] W. Luo, F. Shen, C. Bommier, H. Zhu, X. Ji, L. Hu, Acc. Chem. Res. 49 (2016) 231–240
  - [14] A. Eftekhari, D.-W. Kim, J. Power Sources 395 (2018) 336–348.
  - [15] J.-Y. Hwang, S.-T. Myung, Y.-K. Sun, Chem. Soc. Rev. 46 (2017) 3529–3614.
  - [16] D. Stevens, J. Dahn, J. Electrochem. Soc. 147 (2000) 1271.
  - [17] P. Ge, M. Fouletier, Solid State Ionics 28 (1988) 1172-1175.
  - [18] J. Qian, X. Wu, Y. Cao, X. Ai, H. Yang, Angew. Chem. Int. Ed. 52 (2013) 4633–4636.
  - [19] S. Liu, J. Feng, X. Bian, J. Liu, H. Xu, Y. An, Energy Environ. Sci. 10 (2017) 1222–1233.

#### Y. Shen et al.

- [20] J. Sun, H.-W. Lee, M. Pasta, H. Yuan, G. Zheng, Y. Sun, Y. Li, Y. Cui, Nat. Nanotechnol. 10 (2015) 980.
- [21] L. Li, Y. Zheng, S. Zhang, J. Yang, Z. Shao, Z. Guo, Energy Environ. Sci. 11 (2018) 2310–2340.
- [22] W. Liu, H. Zhi, X. Yu, Energy Stor. Mater. 16 (2019) 290–322.
- J. Ni, M. Sun, L. Li, Adv. Mater. 31 (2019) 1902603.
   J.-Y. Hwang, H.-L. Du, B.-N. Yun, M.-G. Jeong, J.-S. Kim, H. Kim, H.-G. Jung, Y.-
- [24] S.-T. Hwang, H.-E. Du, D.-Y. Hui, M.-G. Song, S.-S. Kin, H. Kim, H.-G. Sung, F.-K. Sun, ACS Energy Lett 4 (2019) 494–501.
   [25] X. Chen, M. Najafi, Solid State Ionics 341 (2019) 115043.
- [26] T. Zhou, W.K. Pang, C. Zhang, J. Yang, Z. Chen, H.K. Liu, Z. Guo, ACS Nano 8
- [20] T. LING, W.K. Fang, C. Zhang, S. Fang, Z. Ghell, F.K. Ed, Z. Guo, Red Natio 6 (2014) 8323–8333.
   [27] C. Ma, J. Xu, J. Alvarado, B. Qu, J. Somerville, J.Y. Lee, Y.S. Meng, Chem. Mater.
- [27] G. May, G. Fart, and G. P. Guy, G. G. Goner, Chine, G. F. Core, F.G. Michell, G. Harris, C. Fart, and C. S. Core, C. S. Core, S. C. Start, and C. S. Core, C. S. Core, S. C. Sand, C
- [20] J. Kin, H. Kun, Z. Mag, M.H. Lee, R. Lin, G. Foon, R. Kang, R.V. Energy Match C (2016) 1600943.
   [29] J. Jiang, J. Zhu, W. Ai, Z. Fan, X. Shen, C. Zou, J. Liu, H. Zhang, T. Yu, Energy
- Environ. Sci. 7 (2014) 2670–2679.
- [30] L. Xiao, H. Lu, Y. Fang, M.L. Sushko, Y. Cao, X. Ai, H. Yang, J. Liu, Adv. Energy Mater. 8 (2018) 1703238.
- [31] H. Hou, X. Qiu, W. Wei, Y. Zhang, X. Ji, Adv. Energy Mater. 7 (2017) 1602898.
- [32] H. Hou, C.E. Banks, M. Jing, Y. Zhang, X. Ji, Adv. Mater. 27 (2015) 7861-7866.
- [33] J. Hou, C. Cao, F. Idrees, X. Ma, ACS Nano 9 (2015) 2556–2564.
- [34] Y. Qie, J. Liu, S. Wang, Q. Sun, P. Jena, J. Mater. Chem. A 7 (2019) 5733-5739.
- [35] J. Liu, X. Li, Q. Wang, Y. Kawazoe, P. Jena, J. Mater. Chem. A 6 (2018) 13816–13824.
- [36] P.E. Blöchl, Phys. Rev. B 50 (1994) 17953.

- [37] G. Kresse, J. Furthmüller, Phys. Rev. B 54 (1996) 11169.
- [38] J.P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. 77 (1996) 3865.
- [39] H.J. Monkhorst, J.D. Pack, Phys. Rev. B 13 (1976) 5188.
- [40] G. Henkelman, H. Jónsson, J. Chem. Phys. 113 (2000) 9978-9985.
- [41] G. Henkelman, B.P. Uberuaga, H. Jónsson, J. Chem. Phys. 113 (2000) 9901–9904.
- [42] S.P. Ong, W.D. Richards, A. Jain, G. Hautier, M. Kocher, S. Cholia, D. Gunter, V. L. Chevrier, K.A. Persson, G. Ceder, Comput. Mater. Sci. 68 (2013) 314–319.
- [43] S. Wang, Q. Bai, A.M. Nolan, Y. Liu, S. Gong, Q. Sun, Y. Mo, Angew. Chem. Int. Ed. 58 (2019) 8039–8043.
- [44] Y. Mo, S.P. Ong, G. Ceder, Chem. Mater. 24 (2012) 15-17.
- [45] X. He, Y. Mo, Phys. Chem. Chem. Phys. 17 (2015) 18035-18044.
- [46] W. Tang, E. Sanville, G. Henkelman, J. Phys. Condens. Matter 21 (2009), 084204.
  [47] M. Mortazavi, C. Wang, J. Deng, V.B. Shenoy, N.V. Medhekar, J. Power Sources 268 (2014) 279–286.
- [48] U. Arrieta, N.A. Katcho, O. Arcelus, J. Carrasco, Sci. Rep. 7 (2017) 1-8.
- [49] Y. Qie, J. Liu, X. Li, S. Wang, Q. Sun, P. Jena, Phys. Rev. Mater. 2 (2018), 084201.
   [50] A. Arico, P. Bruce, B. Scrosati, J. Tarascon, W. Van Schalkwijk, Nat. Mater. 4 (2005) 366–377.
- [51] R. Tripathi, G.R. Gardiner, M.S. Islam, L.F. Nazar, Chem. Mater. 23 (2011) 2278–2284.
- [52] K. Wang, Y. Xu, Y. Li, V. Dravid, J. Wu, Y. Huang, J. Mater. Chem. A 7 (2019) 3327–3335.
- [53] J. Liu, S. Wang, Q. Sun, Proc. Natl. Acad. Sci. Unit. States Am. 114 (2017) 651-656.
- [54] J. Liu, S. Wang, Y. Qie, C. Zhang, Q. Sun, Phys. Rev. Mater. 2 (2018), 025403.
- [55] H. Xie, Y. Qie, M. Imran, Q. Sun, J. Mater. Chem. A 7 (2019) 14253–14259.