First Principles Study on The Electro-Mechanical Properties of Silicon Carbide (Sic) As an Anode for Battery Applications

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Abstract—**First principles study on the electro-mechanical properties of Silicon Carbide (SiC) as an anode for battery application is achieved by performing electronic structure calculations and ab-initio molecular dynamic simulations within the framework of density functional theory run on quantum espresso package. The Silicon Carbide material under study is found to be a semiconductor material with an indirect bandgap of about 2.895 eV implying it has good electronic conductivity. Also, Silicon Carbide has fairly high elasticity value of 503.87 Pa, yield stress value of 11.333 N/m2 and is observed to have large modulus of resilience than modulus of toughness, hence is found to be ductile. Thus, the properties under study are important when the material is to be fabricated /alloyed under controlled techniques by pressing, forging or rolling into a given flat/rod-like design as an anode for battery application.**

Keywords—Electro-Mechanical Properties; Silicon Carbide; Anode; Battery.

I. INTRODUCTION

Conventional Lithium ion Batteries (LIBs) using an anode with Carbon content such as any combination of Silicon(Si)/Graphite(G)/Carbon(C) and lithium transition-metal oxide cathodes are approaching their theoretical energy density due to the constant pressure on the relevant academic and industry communities to improve the energy density of LIBs. The energy density of LIBs is closely related to the electrode materials and their specific capacity. There is more room in anode materials to increase the capacity as compared to cathode materials. For example, the gravimetric capacity of Si anode is 10 times higher than that of conventional graphite anode (372 mAh/g) as found from experimental work [1 & 2]. With the same cathode material in a Lithium(Li) ion battery system, replacing graphite with Si can significantly improve the energy density of LIBs. Therefore,Si has been considered as one of the most promising next generation anodes towards high-energy LIBs because of its high theoretical capacity than that of graphite, low working voltage, and its abundance in the earth's crust [3,4,5]. However, unlike the intercalation-type anodes (eg, Graphite), the alloying/dealloying reaction of Si as an anode with Li induces huge volume changes (>300%). Such huge volume changes during electrochemical cycling will lead to repeated cracking and pulverization of Si, hence the disintegration and fracturing of the Si electrode, accompanied by electrical isolation. The repeated cracking and pulverization will also lead to the continual breaking up of the Solid Electrolyte Interphase (SEI) layer and the explosion of new surface, which will quickly consume the electrolyte and Li ions in the electrolyte.

Therefore, the use of sole Si anode suffers from extremely fast electrolyte decay and low Coulombic Efficiency (CE) as a result of the severe volume changes and unstable SEI films. Design strategies for advanced materials, like creating unique nanostructures and forming composites with electrochemically inactive/less active materials, are academic approaches to significantly improve the cycle life of the LIBs.[6,7,8]

The commercial goal of achieving high-performance anodes to replace the existing commercial Graphite materials with Si or any combinations of Si/G/C , involves reaching a specific capacity and Coulombic Efficiency (CE) [9,10]. Graphite is a low cost commercial anode with high CE, excellent cycle life, good mechanical flexibility, and observed to have only small volume changes when in contact with Li ions in the electrolyte, and has a high electrical conductivity. Research has shown that the use of Si and Graphite has emerged as the most practical anode for high-energy LIBs. With Graphite the preferred choice over Silicon anode because of the high volume changes and unstable Solid Electrolyte Interphase of Silicon anodes leading to a fast reduction of the electrolyte in LIBs over time.

It has being found that the addition of graphite into Si to form a combination of Si and Graphite can buffer the volume change, increase the electric conductivity, and achieve high specific and volumetric capacities at the same time. Implying the combination of Si and Graphite is more desirable as an anode than either graphite or silicon. Therefore , the combination of Si and Graphite consist of two distinct anodes of different materials synthesized into a single composite, retaining the advantages of both materials while minimizing the dis-advantages of both materials securing its success in the anode market with some commercial value [11]. However, it is still a challenge to integrate the Si and Graphite into a single system or composite to obtain the desired performance, since both of these materials are significantly different in terms of their physical and chemical properties.

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Research devoted to improving and achieving high electrochemical performance with the design and development of the combination of Si and Graphite is realized when Carbon additives are added. Carbon is observed to play an important role in integrating the Si and Graphite from many aspects, such as increasing the interface bonding between the Graphite and Si, alleviating the volume variations of Si, and improving the interfacial chemistry, conductivity, and mechanical integration. The review work titled 'The critical role of Carbon in marrying Silicon and Graphite anodes for high-energy lithium-ion batteries' written by Jingxing Wu, Yinliang Cao, Haimin Zhao, Jianfeng Mao, Zaiping Guo, highlighted the critical role of Carbon additives, as well as the associated synthesis methods and structures for achieving high-performance Si/G/C composites for developing high energy-density LIBs, and provided possible insights for the future development of practical Si/G/C composite anodes. To alleviate the drawbacks of any combinations of Si/G/C due to the loose connections among the Graphite particles and the poor interface adhesion between Graphite and Si. There is the need to achieve high-capacity and stable combinations of Si/G/C composite to maximize the benefits of the combination of Si/G/C. This is addressed during the synthesis process by considering the structure, surface morphology of the combination of Si/G/C composite. Addition of Carbon in varying concentration to the combination of Si and Graphite is found to construct the desirable structure and surface morphology with maximum benefits [12,13,14,15,16,17]. Therefore, Carbon additives have been intensively used to prepare the combinations of Si/G/C composites with the formation of new structures and surface modification to maintain high-capacity and long-cycling stability. Efforts have been made to combine different forms of Carbon additives with Si and Graphite to form uniform conductive structures and to prepare Si/G/C composite materials with good electrical conductivity, good adhesion, high chemical stability and high electrochemical performance [18,19]. Optimization of the ratio between Silicon, Graphite, and Carbon materials to obtain the desired structure and surface morphology has been the main focus for the past decade with the purpose of improving the batteries performance with a desired anode made up of a combination of Silicon, Graphite and Carbon.

Despite the high theoretical capacity of Silicon than Graphite which makes Silicon the most promising anode. Its weakness due to severe volume changes during cycling and poor cyclic stability leading to low electrical conductivity over time as the electrolyte decays is attributed to the particle size of Silicon [20,21]. In light of that, ongoing research seeks to reduce the particle size which can be achieved during the synthesis and fabrication stages by doping with carbon while controlling the surface morphology [22,23,24]. In this computational research article, silicon is doped with carbon by the use of optimization ratio and the electro-mechanical properties of carbon doped silicon is studied in relation to its suitability as an anode for battery application.

II. METHODS

A. Electronic Structure Methods

For the electronic structure calculations the total energy, fermi energy, bandgap, energy bands and density of states are achieved with density functional theory within the framework work of projected augmented plane wave basis as implemented on Quantum Espresso Package. The exchange correlation effects are accounted for by using Perdew Burke Ernzerhof(PBE) within the Generalized Gradient Approximation method. The kinetic energy and the charge density cut off is 25.00 Rydberg (Ry) and 100.00 Ry respectively with a convergence threshold of 1.0E-06, mixing beta of 0.7, Ultrasoft plus core correction as Pseudopotential and K-points set to 4x4x4 Meshgrid. The Self Consistent Field(SCF) and the Non Self Consistent Field calculations are run with the optimized settings. High symmetry K-points are calculated to integrate the Brillouin Zone with the 4x4x4 Meshgrid replaced and that settings used in the Bandgap, Energy Bands and Density of states calculations.

B. Molecular Dynamic Simulation Methods

Ab initio molecular dynamic simulation refered to as molecular dynamic simulation from first principles uses parameter free potentials to compute the interatomic forces based on the electronic structure calculation within the framework of Density Functional Theory [25] [26], [27]. This is implemented by setting the calculation to run molecular dynamic simulation for physical properties and setting a time interval of 0.00048 pico-seconds, the number of iteration steps set to 20 and the ionic dynamics set to Beeman as default settings. Interatomic forces such as forces acting on atoms,non-local contrib. to forces,core correction contribution to forces, Hubbard contribution to forces,SCF correction term to forces and stress such as kinetic stress,local stress, nonloc. Stress, hartree stress, exc-cor stress, corecor stress, ewald stress, hubbard stress, london stress, Density Functional Theory Dispersion correction (DFT-D3) stress, Exchange-hole Dipole Moment (XDM) stress, **Density Functional Theory incorporating Non-Local correlation functionals** (dft-nl) stress, Thermal stress within van der Waals materials (T-vdW stress), Three-Dimensional Reference Intereaction Site Model (3D-RISM) stress are computed and displayed. In addition, the average stress value is determined as the trace of the stress matrix by finding one third of the sum of all the diagonal elements of the stress matrix and same done to compute for the average pressure. After each time iteration step, the process is repeated with new force values,stress values,average stress value and average pressure value. After the last iteration step, the data for stress and strain is generated and saved. This is plotted as seen on figure 4a. Labelled Stress verse strain curve.

III. RESULTS AND DISCUSSION

From the computational result of the electronic structure calculations, the Fermi energy of SiC is 27.418 eV and the bandgap of SiC is 2.8953 eV approximately 2.9 eV, implying SiC is a semiconductor material more so with a bandgap of 2.9 eV. From the bandstructure plot on figure 1, SiC is a semiconductor material with an indirect bandgap. From figure 2, the graph of the mean square displacement versus time, the average diffusion coefficient is 0.00119307 cm^2/s and is not same as the Self diffusion coeffiecient, used to determine the ionic conductivity and activation energy as a function of temperature. With suitable electronic and transport properties, SiC can find application in battery studies as an electrode material preferably an anode in a battery system with a suitable electrolyte. SiC has good electronic conductivity since it has a narrow bandgap and hence can conduct electricity easily with an increase in temperature. The valence electrons gain energy and can cross the narrow bandgap into the conduction band from the valence band with an increase in temperature.

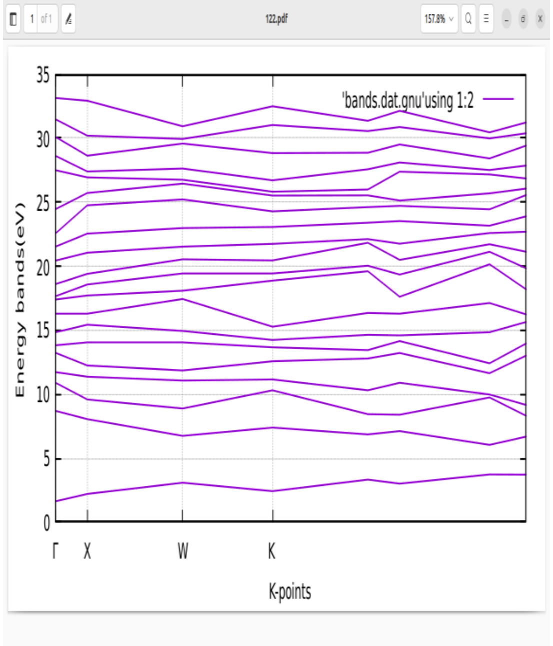

Fig. 1. Bandstructure for SiC

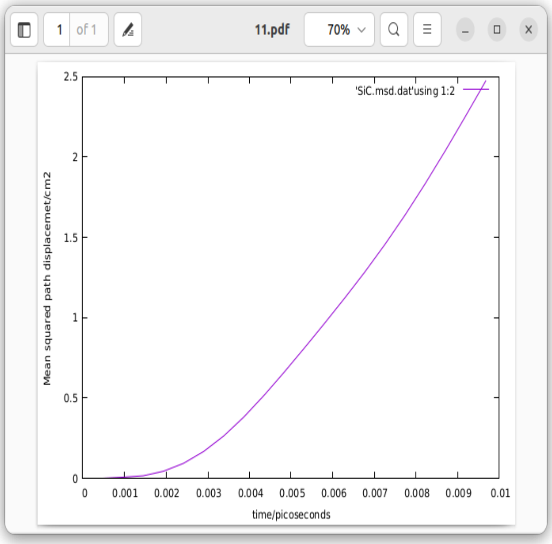

Fig. 2. Mean squared path displacement versus time for SiC

In semiconductor physics, the narrow bandgap represent a barrier that prevents the flow of electrons or holes which constitute the flow of current. If the barrier can easily be overcome then it allows for current to flow through the material without must resistance, hence a good conductor of electricity.

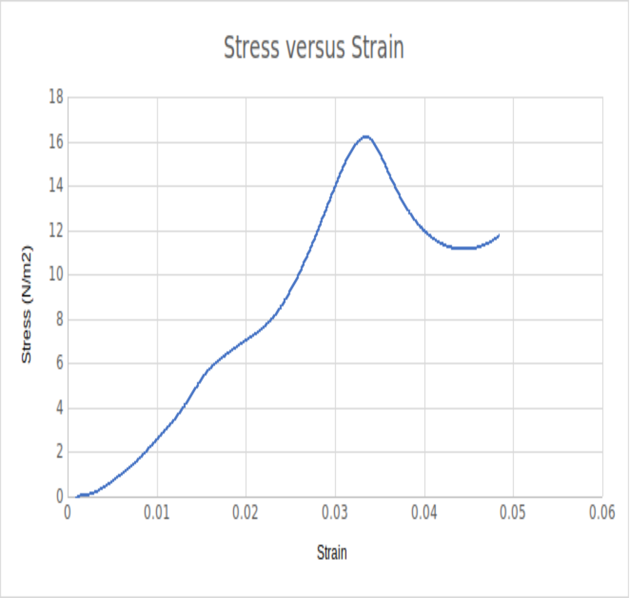

Fig. 3a. Stress verse Strain curve.

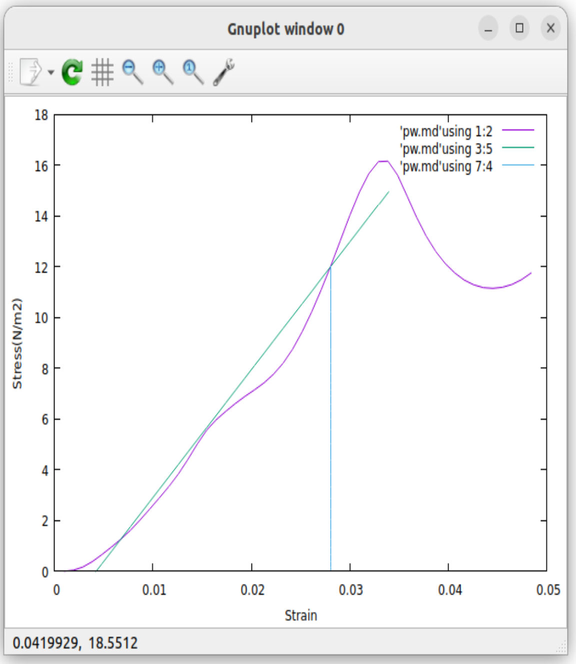

Fig. 3b .Stress verse Strain curve, Region A is Elastic region and B is the Plastic region.

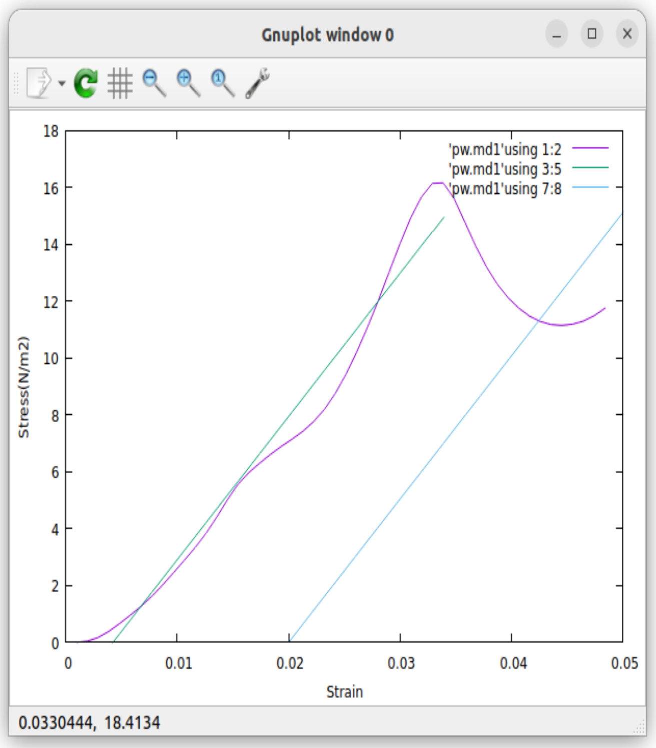

Fig. 3c. stress verse strain curve showing 2 percent offset line.

The area under the linear curve labelled A on figure 3b., is the Elastic region, in this region Hooke's law is obeyed and when the load that causes the stress is removed the material returns to its original form. There is a linear relationship between the stress and the strain and the constant of proportionality is the Young's modulus found to be 503.87 Pa. The linear line whose slope is the Young's modulus or modulus of Elasticity is drawn as a tangent line touching the stress versus strain curve on the fairly linear portion of the curve as seen on figure 3b. On the figure 3c., 2 percent off set line is plotted, this is the parallel line on the figure 3c. The slope on the parallel line is the same as Young's Modulus and the line cuts the stress vs strain curve at a yield stress value. From the 0.02 off set line drawn, the yield stress value is found to be 11.3329 N/m2. This yield stress value is obtained by drawing a horizontal line that cuts the stress axis from the point on the curve where the 0.02 offset line intersect the curve. It can be observed on the fairly linear portion of the curve beyond the value of yield stress, the material loses its elastic behaviour and is said to be permanently deformed because any further strain the material does not return to its original form. The material is then said to have plastic-like behaviour when deformed (i.e in the plastic region, B on figure 3b.) as a result of permanent dislocations in the structure of the material due to strain. A horizontal line drawn as a tangent line that touches the highest point on the curve known as the Ultimate Tensile Strength cuts the stress axis at a point whose value is recorded as the Ultimate stress found to be 16.15 N/m2. Beyond the Ultimate Tensile strength and for that matter the Ultimate stress value, any further strain hardening reduces the stress as seen on the curve and the material is said to have some further deformation in the plastic region resulting in a smaller and smaller cross-sectional area despite an increase in length of the material. This means beyond the Ultimate Tensile Strength necking begins till the material fractures. Fracture is said to occur at the point at which the material breaks into two or fails which is the last point on the stress versus strain curve with a fracture stress value of 11.746 N/m2. A vertical line drawn from the point on the stress versus strain curve known as Ultimate Tensile Strength cuts the strain axis at an Ultimate strain value. The area under the curve beginning from the first point on the curve to the vertical line described is the Modulus of Resilience. Also, the area under the curve beginning from the fracture point on the curve to the vertical line is the Modulus of Toughness. On the stress versus strain curve, it can be seen that SiC has a large Modulus of Resilience as compared to the Modulus of Toughness. This implies SiC is not too tough but with some considerable resilience, hence SiC is ductile.

IV. CONCLUSION

The Silicon Carbide material under study was found to be a semiconductor material with an indirect bandgap of about 2.9 eV and an average diffusion coefficient of 0.0011937 cm2/s as obtained from the electronic structure information on figure 1 and the graph on figure 2 obtained from the Ab-initio molecular dynamic simulation. This implies Silicon Carbide can find application in battery studies as an electrode material preferably as anode since it has good electronic conductivity. With regards to the mechanical property of Silicon Carbide, it is observed from the stress verse strain curves on figure 3a, 3b and 3c. Silicon Carbide has an elasticity modulus of about 503.87 Pa and a yield stress value of 11.3329 N/m2; beyond this yield stress value Silicon Carbide is said to be permanently deformed and below this value Silicon Carbide is said to have an elastic behaviour. The value of yield stress is important in structural engineering when the material under study is alloyed/dealloyed/fabricated under controlled techniques by pressing, forging or rolling into a given flat/rod-like design as anode for battery application. Any further strain when Ultimate Tensile Strength is reached necking is said to occur till Silicon Carbide fractures. Silicon Carbide is observed to have large Modulus of Resilience than Modulus of Toughness and is found to be Ductile.

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REFERENCES

[1] Liang B, Liu Y and Xu Y J. Power Sources 2014, 267, 469–90, doi:10.1016/j.jpowsour.2014.05.096

[2] Liu N, Lu Z, Zhao J, McDowell M T, Lee H W, Zhao W and Cui Y Nat. Nanotechnology. 2014, 9, 187–92, doi: 10.1038/nnano.2014.6

[3] Jin Y, Zhu B, Lu Z, Liu N, Zhu J. Adv Energy Mater. 2017;7(23):1700715,doi: 10.1002/aenm.201700715

[4] Q. Ji, J. Qing, Y. Xia, J. Zhu, B. Hu, P. M-Buschbaum, Ya-J. Cheng, Practically Relevant Research on Silicon-Based Lithium-Ion Battery Anodes 2019,https://doi.org/10.1002/9781119407713.ch5

[5] Choi M, Lee E, Sung J, N. Kim,M. KoNano Research, 2024, 17(6): 5270-5277. https://doi.org/10.1007/s12274-024-6512-x

[6] Luo W, Chen X, Xia Y, et al. Adv Energy Mater. 2017;7:1701083.,doi:10.1002/aenm.201701083

[7] Zhu G, Zhang F, Li X, et al. Angew Chem, Int Ed. 2019;58:6669-6673.,doi: 10.1002/anie.201902083

[8] Luo W, Wang Y, Chou S, et al. Nano Energy., 2016;27:255-264, doi: 10.1016/j.nanoen.2016.07.006.

[9] Chae S, Choi SH, Kim N, et al. Angew Chem. 2019. https://doi.org/10. 1002/anie.201902085.

[10] S. Zhu,J. Zhou,Y. Guan,W. Cai,Y. Zhao,Y. Zhu,L. Zhu,Y. Zhu,Y. Qian, 2019, PubMed 14(47), doi: 10.1002/smll.201802457

[11] N. Kim, C. Oh, J. Kim, J-Soo Kim, E. D. Jeong, J-Seong Bae, T. E. Hong and J. K. Lee, 2017 J. Electrochem. Soc. 164 A6075, doi:10.1149/2.0101701jes

[12] Liu X H, Zhong L, Huang S, Mao S X, Zhu T and Huang J Y, ACS Nano 2012, 6, 1522–31.doi: 10.1021/nn204476h

[13] Liu W, Xu H, Qin H, Lv Y, Zhu G, Lei X, Lin F, Zhang Z and Wang L, J. Mater. Sci. 2020, 55, 4382–94. https://doi.org/10.1007/s10853-019-04313-x

[14] Chen H, Hou X, Chen F, Wang S, Wu B, Ru Q and Qin H, Carbon 2018, 130, 433–40. doi:10.1016/j.carbon.2017.11.013

[15] Chen H, Wang Z, Hou X, Fu L, Wang S, Hu X, Qin H, Wu Y and RuQ,Electrochim.Acta2017,249,113–21.doi:10.1016/j.electacta.2017.07.146.

[16] Ru H, Xiang K, Zhou W, Zhu Y, Zhao X S and Chen H, Electrochim. Acta 2016, 222, 551–60,doi: 10.1039/c5gc02122g

[17] Zhou M, Li X L, Wang B, Zhang Y B, Ning J, Xiao Z C, Zhang X H, Chang Y H and Zhi L J, Nano Lett. 2015, 15, 6222–8. doi:10.1021/acs.nanolett.5b02697

[18] Kim SY, Lee J, Kim BH, Kim YJ, Yang KS, Park MS.ACS Appl Mater Interfaces. 2016 May 18;8(19):12109-17. doi: 10.1021/acsami.5b11628

[19] Lin N, Xu T, Li T, Han Y, Qian Y.ACS Appl Mater Interfaces. 2017 Nov 15;9(45):39318-39325. doi: 10.1021/acsami.7b10639.

[20] Y. Bai , X. Cao, Z. Tian, S. Yang and G. Cao NanoExpress 2(2021) 010021 https://doi.org/10.1088/2632-959X/abdf2e.

[21] Zuo X, Zhu J, Mü ller-Buschbaum P and Cheng Y, Nano Energy 2017, 31, 113–43. https://doi.org/10.1016/j.nanoen.2016.11.013

[22] Wang M S, Song W L, Wang J and Fan L Z, Carbon 2015, 82, 337–45.doi: 10.1016/j.carbon.2014.10.078

[23] Chae S, Ko M, Kim K, Ahn K and Cho J, Joule 2017, 1, 47–60, doi: 10.1016/j.joule.2017.07.006.

[24] Y. Bai, X. Cao, Z. Tian, S. Yang and G. Cao, 2021 Nano Ex. 2 010021,DOI 10.1088/2632-959X/abdf2e

[25] M. Meyer and V. Pontikis (eds.), Computer Simulation in Materials Science, 283-304.© 1991 Kluwer Academic Publishers. DOI:10.1007/978-3-319-01905-5_60-2

[26] R. N. Abugre, S. A. Atarah, G. G. Hagoss, and R. N. Abugre, “Ab Initio Molecular Dynamic Simulation of the Ionic Transport Mechanisms for LiCoO2 and Ni Doped LiCoO2 as Cathodes in Lithium Batteries,” *J. Physico-Chemical Mater.*, vol. 1, no. 1, pp. 13–18, 2024, doi: 10.64820/AEPJPCM.11.13.18.122024.

[27] R. N. Abugre, S. A. Atarah, G. G. Hagoss, and R. N. Abugre, “First Principles Study on the Structural and Electrochemical Properties of LiCoO 2 and Ni Doped LiCoO 2 Cathodes in Lithium Batteries,” *J. Physico-Chemical Mater.*, vol. 1, no. 1, pp. 7–12, 2024, doi: 10.64820/AEPJPCM.11.7.12.122024.