

# The economic and management use of rhododendron petals in potas-sium-ion nano batteries anode via efficient computer simulation

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**Abstract.** Nano batteries are manufactured batteries which use nanoscale technology, small particles measuring less than 100 nanometers or 10<sup>-7</sup> meters. In addition, because of plentiful potassium supplies and less cost, potassium-ion batteries (PIBs) are taken as possible substitutes for lithium-ion batteries for massive energy storing systems. Our modern lifestyle could be totally different without rechargeable batteries. Regarding their economic and management usage, these batteries are applied in electric and hybrid vehicles, devices, and renewable power generation systems. Accordingly, regarding the huge K ion radius, it is a difficult process for identifying relevant materials with excellent cycling stability and capacity. At present, the production of suitable anode materials with high specific capacities, long cycle life and low costs for PIBs remains a major challenge. Also, the continuing improvement in defining future electors, the manufacture of PIBs has been complicated by multiple challenges, namely low reversible performance, insufficient cycling stability and poor energy density, all of which have created important doubts for the effective implications of PIBs. Nano-particles have shown various advantages for enhanced energy and power density, cyclability and safety when it comes to designing and producing electrode materials via efficient computer simulation. In combination with large volume expansion, slow reaction kinetics, and low electrical conductivity the main cause for the degradation of SnO<sub>2</sub> reaction reversibility and power decay observed are not as obvious as those of Lithium-ion batteries (LIBs) as anodes of sodium-ion batteries (SIBs), and potassium-ion batteries (KIBs).

**Keywords:** biomass; hard carbon; potassium-ion batteries; nitrogen-doped; energy storage mechanism

## 1. Introduction

In 2018, the global demand for energy storage was estimated at \$72 billion and is projected to rise to \$165 billion before 2025 (Dyatlov *et al.* 2020). The global battery market has been estimated to be progressed by 6.63% CAGR during the expected years of 2019-27 (Baumann *et al.* 2021). In addition, the energy crisis on Earth is disrupting the growth and creating difficulties for human survival (Mehtab *et al.* 2019, Yang *et al.* 2020a, Yasin *et al.* 2020). The need for physically small batteries is growing rapidly with the growth in need for portable electronics (Shi *et al.* 2020, Fujita *et al.* 2021, Zhang *et al.* 2021). Thus, the miniaturization of the battery is a critical task that the

battery community must take into account. For especial purposes, namely micro-electromechanical systems and chips, nano-scale batteries are used extensively (Chen *et al.* 2018, Lei *et al.* 2020). Regarding the use of computer simulation, nano battery incorporated in device indicates that power sources are also important in the process of miniaturization. The key characteristics of Nano batteries with dimensions of 1 cm<sup>2</sup> (Lowy *et al.* 2008) are their energy and power densities. When these tiny devices are integrated in parallel, then thousands of Nano batteries could be placed on 0.5-mm-thick substrate which can have a charge of up to 10-mAh cm<sup>2</sup> power per footprint. These batteries were evaluated for a significant number of charge-discharge rounds, without compromising their stability and capacitance. In addition, this design provides a massive electrical power output that eliminates the risk of flammability, a big source of malfunctioning in laptop and mobile batteries. Novel battery technologies in nano world

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allow Nano battery systems to stay operational for a minimum duration of 15 years (Ni *et al.* 2019a, b, Ning *et al.* 2020). The advancement of energy storage systems by waste management focuses on advanced energy technology. The lightweight N-S doped carbon nanofibers as hybrid condensers would be promoted by it. The satisfactory electrochemical results encourage the principle of waste management in order to scalable energy storage device efficiency (Zuo *et al.* 2015, 2017, Zhang *et al.* 2020a). The Nano battery can apply both to Nano sized batteries, as well as to the use of macroscopic battery nanotechnology to improve its efficiency and lifespan (Rouhanifar *et al.* 2019, Hu *et al.* 2020, Yang *et al.* 2020b). Nano battery can deliver many benefits, including fast charging, higher power density, and prolonged shelf life over the conventional battery (Guo *et al.* 2020, Wang *et al.* 2020, Yan *et al.* 2021). For a primary (non-rechargeable) battery, it is possible to use nanotechnology to obtain a high-performance primary battery. Iost *et al.* (2016) stated using monolayer graphene to provide an initial battery on a chip. For several hours, their batteries produced a steady voltage (1.1 V) with a high 15  $\mu\text{Ah}$  power. Nano- $\text{MnO}_2$  was utilized as a cathode material (Srither *et al.* 2013) to improve the discharge power and energy density of magnesium primary batteries. Srither *et al.* (2014) published similar findings in the primary cell of  $\text{Zn/MnO}_2$  for the improvement of discharge power retention and shelf life. In the high-power alkaline  $\text{Zn-MnO}_2$  batteries (Cheng *et al.* 2005),  $\gamma\text{-MnO}_2$  nanowires/nanotubes could be used. The multi-walled carbon nanotube (MWCNT)-templated cobalt phthalocyanine (CoPc) can increase its discharge energy as a catalyst for the  $\text{Li/SOCl}_2$  battery (Xu *et al.* 2010). Wei *et al.* (2017) manufactured a hybrid nanomaterial (acetylene black nanoparticles/graphene nano sheets) as a high-discharge  $\text{Li/SOCl}_2$  battery cathode material (1706  $\text{mAh/g}$  capacity at 5  $\text{mA/cm}^2$  current density). Sun *et al.* (2016) developed an electrode on the basis of nano-V, Ti-doped  $\text{MnO}_2$  for high-rate batteries for the  $\text{Li-MnO}_2$  battery. For secondary (rechargeable) batteries, Douglas *et al.* (2015) have suggested that the sodium-sulfur and lithium-sulfur conversion reactions for successful batteries were improved by  $\text{FeS}_2$  nanoparticles (4.5 nm). The author stated that while conversion reaction was occurring, the scale of the nanoparticles was close to the diffusion length of iron, hence resulting in reversible and efficient cation trades. The insertion of nano- $\text{Al}_2\text{O}_3$  particles into the sulfur electrode in the lithium/sulfur battery not only stopped the breakdown of lithium polysulfides into liquid electrolytes, facilitated the redox reaction of lithium/sulfur (Choi *et al.* 2007, Liu *et al.* 2021). Various nanomaterials like nano-Si (Teki *et al.* 2009, Yoo *et al.* 2013), C/Si nanocomposite (Si *et al.* 2009), grapheme (Kim *et al.* 2011a, b), nano-SnO (Li *et al.* 1999),  $\text{ZnMn}_2\text{O}_4$  nanowires (Kim *et al.* 2011c), core-shell Sn@Cu nanoparticles (Kim *et al.* 2010), nano- $\text{TiNb}_2\text{O}_7$  (Tang *et al.* 2013), antimony hollow Nano spheres (Hou *et al.* 2014), nano-Sb (He *et al.* 2014), nano- $\text{ZnFe}_2\text{O}_4$  (Xing *et al.* 2012),  $\text{MoO}_3$ /conducting polymer nanocomposite (Liu *et al.* 2014, Habibi *et al.* 2019a), and nano-Al (Sharma *et al.* 2013) have been used regarding to nanostructured anodes in rechargeable batteries. In addition to the experimental

studies and numerical analysis, Artificial intelligence (AI) as one of the accurate, fast and cost-effective techniques have been deployed extensively in different applications (Safa *et al.* 2020, Shariati *et al.* 2020d, Yazdani *et al.* 2020). Machine learning (ML) can be used as a subset of AI to optimize and predict the performance of battery systems (Mohammadhassani *et al.* 2013, Safa *et al.* 2016, Toghroli *et al.* 2016, Mansouri *et al.* 2019). ML also can provide self-learning from data and then without human interference apply that learning. In fact, big data techniques and ML methods have addressed the different problems of modelling the relationship between complex physical characteristics and material properties (Mohammadhassani *et al.* 2014b, Chahnasir *et al.* 2018, Sedghi *et al.* 2018, Katebi *et al.* 2019). Moreover, with the ongoing progress of theories and methods, the subjects in which ML can be employed will be more widespread and have a growing influence on the effectiveness of the investigations (Shariati *et al.* 2019d, e, Trung *et al.* 2019a, Huang *et al.* 2021). Clean and green technology, for example solar, wind, tide, and geothermal has a significant role in recognizing the improvement of human society because of the reduction of environmental destruction, and fossil fuels, thereby becoming the fastest-growing renewable energy alternatives (Shariati 2020, Shariati *et al.* 2020c, f, Rajaei *et al.* 2021). These renewable energies, though, are also essentially intermittent, leading in a tension between the time and space dimensions of energy harvesting and consumption (Naghypour *et al.* 2020a, Shariati *et al.* 2020a, g). To this end, an efficient resolution for storing and distributing these transient energies is known to be the Energy Storage System (ESS) (Shariati 2008, Safa *et al.* 2019, Naghipour *et al.* 2020b, Shariati *et al.* 2020b). LIBs are the prevalent ESS technology at present and, due to their ease, high energy densities and shortage of memory feature have become important in our lives (Shariati *et al.* 2019a, 2020e, Afshar *et al.* 2020). With a gradual increment in LIB uses, due to the relative shortage (0.0017 wt percent in the Earth's crust) and inconsistent lithium source allocation, LIBs could rarely fulfill the growing demand for the future ESS (Chen *et al.* 2019, Shariati *et al.* 2019c, Trung *et al.* 2019b). As a probable alternative to LIBs, due to their low cost, and high sodium availability in the Earth's crust, SIBs have acquired a lot of interest. However,  $\text{Na/Na}^+$ 's comparatively high-standard redox potential (-2.71V vs. the standard hydrogen electrode) [SHE] contributes to the lower energy density of SIBs than that of LIBs, allowing their use in portable electronics and electric cars. Compared to KIBs and SIBs, LIBs have three major potassium advantages. One of these advantages is  $\text{K/K}^+$ 's smaller standard redox potential (-2.93V vs SHE), being much similar to that of  $\text{Li/Li}^+$  (-3.04V vs SHE). This feature allows KIBs to have an energy density that is potentially higher than SIBs. Another advantage is having a lower cost of KIBs because of the high amount of potassium in the Earth's crust. Lastly, the weaker Lewis acidity and the corresponding lower  $\text{K}^+$  radius of Stokes than those of both  $\text{Li}^+$  and  $\text{Na}^+$  can result in the electrolyte's maximum conductivity and ion mobility of  $\text{K}^+$ . It should, however, be acknowledged that four major issues are still present in the latest developments of KIBs.

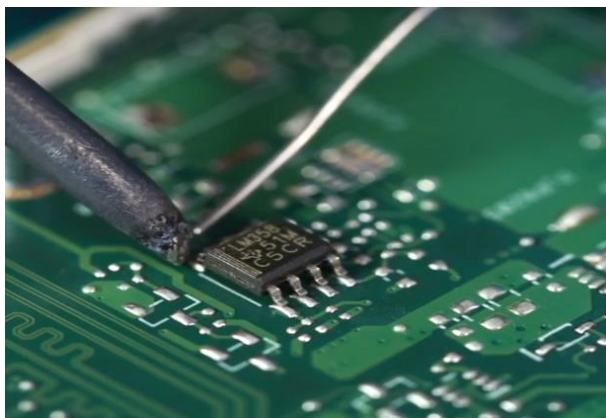


Fig. 1 Micro batteries

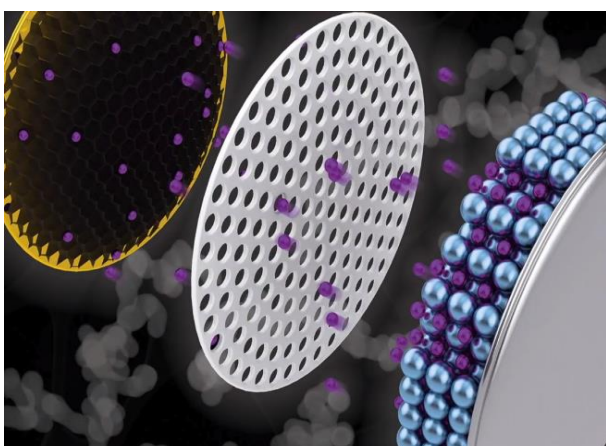


Fig. 2 The structure of batteries

First of all, there is still a shortage of KIB electrodes with high ability to ensure high energy density. Secondly, the rate of function of KIBs is constrained by the comparably low diffusivity in solid electrodes of strong  $K^+$  ions. Thirdly, since the solvent in the electrolyte is more readily decreased on the surface of electrode, the low electrochemical capacity of  $K^+/K$  leads to more side reactions. Ultimately, the electrode materials of KIBs typically are affected by pulverization-induced power fading, leading from a large volume expansion along the phase of potassium ion/ de potassium ion which are often plagued by large  $K^+$  ions. Several research efforts are concerned with figuring out the electrochemical method to effectively address of these issues and to significantly increase the efficiency of KIB energy storage to meet these obstacles (Chernogorov *et al.* 2017, Cao *et al.* 2020b, Chen *et al.* 2020, Liu *et al.* 2020). The production of low-cost and high-performance battery structures are needed in order to meet the increasing requirements for power sources in electric vehicles, handheld devices, and massive energy storage cases (Zhang *et al.* 2020b, c, Kang *et al.* 2021). At the present time, the market is predominantly controlled by lithium-ion batteries (LIBs); but the sustainable usage of LIBs, given the shortage and increasing prices of lithium resources, raises major concerns for the near future (Shariati 2013, Suhatrio *et al.* 2019, Toghrli *et al.* 2020).

A search for possible options as substitutes for LIBs has

been motivated due to the mentioned concerns. Hence, recently, batteries based on earth-rich components have gained a lot of attention, namely Mg-ion batteries, Na-ion batteries (NIBs),<sup>-</sup> and Al-ion batteries. Additionally, Potassium has desired characteristics in usage of battery, including high voltage and decent rate capability, which is found in abundance and is a low-cost element. Some attempts were done for creating KIBs. Latest KIB researches were primarily focused on the creation of carbon-based anodes, comprising graphite, carbon nanofiber, hard carbon, and graphene (Yu *et al.* 2020, Zuo *et al.* 2020, Lei *et al.* 2021). Whilst, the broad potassium ion radius (1.38 Å) makes it challenging for potassium ions to be introduced into intercalation-type electrodes, thus limiting the usage of these anodes to KIBs. The alloying mechanism, driven by information of LIBs, may be a possible way of solving this topic (Toghrli *et al.* 2017, Milovancevic *et al.* 2019, Sajedi *et al.* 2019). Nevertheless, for KIBs, alloying-type anodes have not been investigated frequently. Sn could make various alloys with K in the binary phase diagram as a frequently researched anode with impressive function in NIBs and LIBs, indicating the possible use of Sn and Sn-based materials in KIBs. Sultana *et al.* recently stated a 150 mAh/g capacity for Sn-based nanocomposite anodes in KIBs, albeit with a rapid decline in capacity. Moreover, for Sn anodes in KIBs, a complete description of the degradation and reaction method has not been published. For the production of Sn and other alloying-type anodes for high-function KIBs, a thorough understanding is necessary. An analysis of the electrochemical function, degradation, and reaction methods of Sn nanoparticles in KIBs applying electrochemical in situ Transmission Electron Microscopy (TEM) testing is mentioned in this paper by using computer simulation, which offers a complete approach to learn the basic science of KIB alloy-type anodes. For KIBs, Sn nanoparticles offer a high capacity of 197 mAh/g but easily decay. In situ TEM, electrochemical research shows that Sn nanoparticles' electrochemical potassium ion occurs in a two-step process with KSn alloy emerging after complete reaction, while during de-potassium, nanostructured pores development is completely recoverable during cycling. However, in a few cycles, substantial pulverization happens in the anodes, negatively affecting stability in the cycle. Computer simulation is considerably used to support the control and production planning as the main parts of the digital company. The simulation enables the imitation of a suggested solution to delineate the parameters of a system to gain the needed goals. For companies, simulation is to raise the specific processes and management, also it helps to imitate the efficiency, process in production area etc. The software solution works by the proposal of conceptual model with the related data. After that, a mathematical-logical model was generated that is served as a direct base for realization of simulation model. The behavior and structure of suggested entities need to imitate those of real objects and of the whole system. Subsequently, the realized logical model could be reflected into the selected simulation software. The generation of simulation model is based on the method that is closely related to the selected software solution.

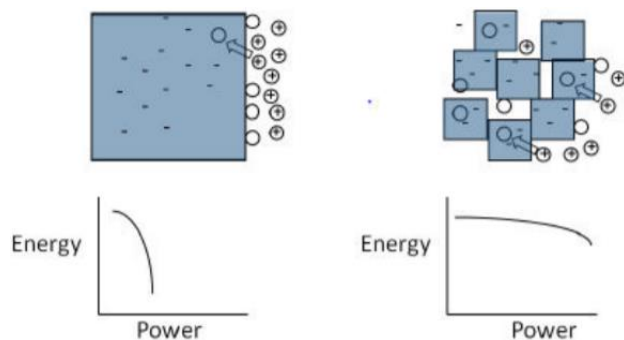


Fig. 3 Chemical reaction and energy/power balance of standard battery vs. Nano phosphate battery

Metal oxides ( $\text{SnO}_2$ ,  $\text{TiO}_2$ ,  $\text{MoO}_2$ , etc.) have the benefits of environmental friendliness, plentiful natural sources, and high theoretical particular capability as a promising anode material for alkali metal ion batteries. In the past few years, they have gained the interest of significant number of researchers.  $\text{SnO}_2$ , an essential member of metal oxides, was researched for LIBs and Sodium Ion Batteries (SIBs) as an anode element. However, fewer studies have been done to date on the K storage efficiency of  $\text{SnO}_2$ . It should be noted that  $\text{SnO}_2$  has the drawbacks of less conductivity, weak reversibility and large volume change that have a significant effect on its reversible specific capacity and cycle stability, therefore affecting its practical value. The researchers improve  $\text{SnO}_2$  with a conductive material (carbon material) or design special structures by new methods of synthesis to solve the above shortcomings in order to achieve excellent electrochemical efficiency. The carbon material will have a decent conductive network to increase the electronic conductivity of the overall electrode and to buffer the volume changes of  $\text{SnO}_2$  along the electrode. While the methods above have significantly improved the electrochemical efficiency of  $\text{SnO}_2$ , there are still a number of issues with the practical application of  $\text{SnO}_2$ . The  $\text{SnO}_2$  composites are generally combined with a conductive agent and a binder for coating on the metal current collector to act as the battery electrode for traditional powder electrode material. As a result, the inactive components substantially decrease the energy efficiency of the battery (current collectors and binders). Furthermore, the contact area of the traditional electrode between active material and electrolyte is small that is not conducive to the maximum application of the active material. In the end, in a repeated cycling process, the enormous volume changes of  $\text{SnO}_2$  electrode resulted in electrode pulverization and escape, leading to rapid decay of capability and low performance. Consequently, it could be an impressive method of enhancing the overall function of  $\text{SnO}_2$  to build binder-free, freestanding three-dimensional (3D) electrodes. In this research, as a freestanding anode for K storage, we anchor  $\text{SnO}_2$  nanoparticles on 3D carbon foam ( $\text{SnO}_2@\text{CF}$ ) via a simple electrodeposition process. The freestanding  $\text{SnO}_2@\text{CF}$  electrode obtained possesses a 3D conductive network, a large electrolyte contact area and supported  $\text{K}^+$  transfer.  $\text{SnO}_2@\text{CF}$  takes significant specific capacity, excellent cycle stability and rate performance in

PIBs, benefiting from the above mentioned characteristics. In addition, via ex-situ XPS, XRD and TEM, the phase transition of  $\text{SnO}_2@\text{CF}$  during charge and discharge processes is seen. Nano batteries are manufactured batteries which use nanoscale method, a scale of minuscule particles measuring less than 100 nanometers or  $10^{-7}$  meters. The anode is almost always graphite, so the cathode and electrolyte materials are often researched (Shah *et al.* 2016a, Nosrati *et al.* 2018). Higher conductivity can be accomplished by shrinking the size of the materials included in a Nano battery, resulting an improved power, both in charge and discharge (Shariati *et al.* 2011, Shah *et al.* 2015, Ziaei-Nia *et al.* 2018, Habibi *et al.* 2019b). Some technologies are predominantly used in Nano batteries: 1) Nano phosphate technology 2) Nano pore battery technology and 3) Lithium ion battery technology (using lithium titanate). An advanced battery system's overall performance and reliability is highly dependent on the chemistry used in the cell (Arabnejad Khanouki *et al.* 2010, 2011, Ismail *et al.* 2018). It is not necessary to mistake nano phosphate with regular lithium iron phosphate (LFP), which has a less capacity and power rate. Nano phosphate is a cathode of lithium ion batteries developed by Professor Todming Chiang and his team (Jalali *et al.* 2012, Davoodnabi *et al.* 2019, Xie *et al.* 2019). The particles of Nano phosphate are classified into two sets, i.e., Primary and also secondary. Chemical reactions provided by monophosphate technology, on the other hand, raise the cathode surface area of the electrolyte, allowing faster incorporation of lithium and leading to more power (Wei *et al.* 2018). Also, much of the bulk volume is still applied to store resources.

The persistent power capacity over a wide span of states of charge is another important aspect of Nano phosphate technology (SOC) (Mohammadhassani *et al.* 2014a, Li *et al.* 2019, Luo *et al.* 2019). At low SOC, majority of battery technologies have considerably lower power capabilities. Nano phosphate has outstanding abuse properties. Both of the lithium ions are moved throughout the full charge/discharge case in these chemistries (Hamidian *et al.* 2011, Shariati *et al.* 2018, 2019b). In majority of cathode metal oxide materials, particularly materials based on cobalt and nickel, only half of the lithium available is moved along normal activity (Shariati *et al.* 2010, Shah *et al.* 2016b, Shahabi *et al.* 2016). Since metallic lithium is far more reactive than ionic lithium, the consequence is that the lithium plates on the anode's surface produce risks (Daie *et al.* 2011, Mohammadhassani *et al.* 2014c, Nasrollahi *et al.* 2018). Since all the lithium ions in nano phosphate chemistry are transferred during charging to anode, during an overcharge case, it is far less common for lithium metal to plate on the anode surface (Afsar Dizaj *et al.* 2018, Al Kajbaf *et al.* 2018, Asadolahi *et al.* 2020, Rouhanifar *et al.* 2020). Usually, cycle life is characterized as the number of incidents a battery could be discharged and charged until its capacity falls below 70 to 80% of its original capacity or energy from the nameplate (Fanaie *et al.* 2014, 2015, 2016). Earlier, by positioning two electrodes inside a nanopore (made of anodic aluminum oxide) and utilizing ultra-thin electrical insulating material to isolate them, researchers

created 3-D nanostructured batteries (Goudarzi *et al.* 2016, Jahanbakhti *et al.* 2017, Ghanbari-Ghazijahani *et al.* 2020). This device has enhanced power and energy density, utilizing these thin electrical insulators restricts the retention of charge and involves complex circuits to transfer current between them (Qi *et al.* 2019, Majedi *et al.* 2020, Qi *et al.* 2020). However, due to spatial constraints of the material, it is hard to maintain the advantages of the 3-D nano-architecture. Liquid formulas of electrically conductive ions (electrolytes) were applied to connect battery circuits, rather than using wired circuits. On the other hand, nano-batteries that apply electrolytes displayed low charge storage (Ngo *et al.* 2018, Alaskar *et al.* 2020b, Cao *et al.* 2020c, Majedi *et al.* 2021). Additionally, uneven ion concentration gradients were led to uneven current densities when used in combination with 3-D structures. Recently, via the design of a battery that incorporates many components more efficiently, researchers have addressed these constraints (Han *et al.* 2018, Dinh-Cong *et al.* 2019, Alyousef *et al.* 2020, Huang *et al.* 2020). A parallel set of Nano batteries make up the latest battery design. All nanotubes include electrodes and liquid electrolytes situated in a nanopores made of anodic aluminum oxide. Each nanotube consisted of a current collector made as the energy storage material by an outside nanotube of an inner nanotube of  $V_2O_5$ . Every end of the nanopore was either coated with  $V_2O_5$  or with a chemically changed form of  $V_2O_5$  to act as the cathode and anode electrodes (Alaskar *et al.* 2020a, Cao *et al.* 2020a, d, Chowdhury 2021). The output of both individual electrodes was calculated. Both implementations demonstrated excellent preservation of electrical storage and a long lifetime charge-discharge cycle. This nanopore battery has triple the electrical storage capacity and an order of magnitude longer cycle life in comparison to prior nanowire battery devices utilizing the same material. The superior cycle lifetime is attributed by researchers to the coaxial tubular structure. The design of the nanotube was found to have a far higher electrical storage potential than the planar structure. These authors have shown that appropriately scaled nanostructures are a viable alternative for enhanced structures of batteries. This unique structure could be a choice for potential portable devices, including phones, tablets, and more, with an improved discharge lifetime and cycle lifetime.

## 2. Nano-structured battery

The specifications such as longer life, stability, remote UPS (uninterruptible power supply) applications are not fulfilled by lead-acid battery technology, and traditional Li-ion technology. Furthermore, abusive conditions such as short circuit, over recharge, exposure to excessively high or low temperatures, over discharge could not be tolerated by these technologies. Using nanotechnology, ALTAIRNANO designed a novel battery and reducing certain disadvantages of traditional designs. The Li-ion technology of ALTAIRNANO is different from the widely applied Li-ion model. They substituted the graphite material with nano-structured lithium titanate that is used in traditional batteries.

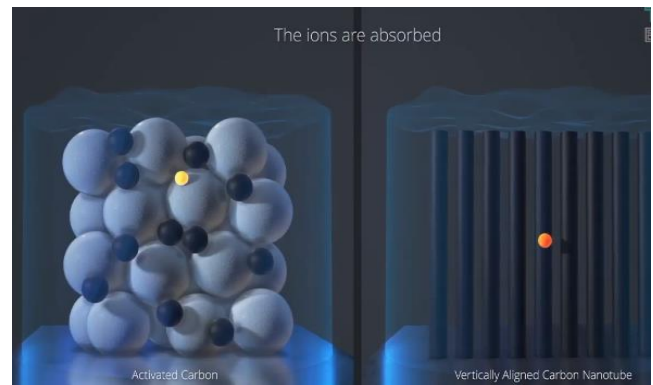


Fig. 4 Traditional Li-ion technology

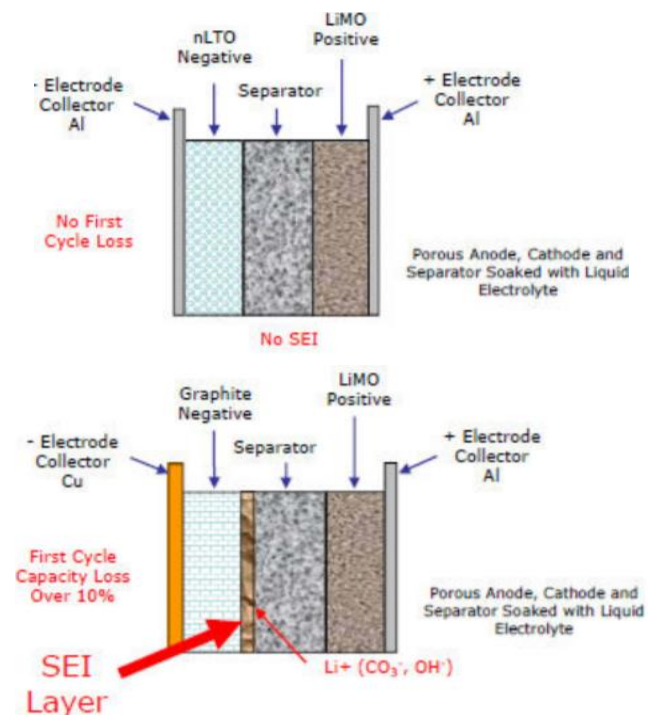


Fig. 5 Comparing of Nano structured battery (Fig. 1) and traditional graphite

## 3. Methodology preparation of $\text{SnO}_2/\text{SSM}$

A hydrothermal process was used to produce the  $\text{SnO}_2/\text{SSM}$  products. Especially, to ready the precursor solution, NaOH (1.2 g) and  $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$  (3.4 g) were added at room temperature in 40 mL deionized (DI) water. The SSM was applied to the hydrothermal reaction precursor solution after ultrasound washing in dilute hydrochloric acid, DI water, ethanol and acetone, respectively. The mix has been moved into an autoclave of Teflon-lined stainless-steel and cooked (24 h) at  $200^\circ\text{C}$ . After treating the SSM with ethanol and DI water (5 times),  $\text{SnO}_2/\text{SSM}$  was extracted. During the processing of  $\text{SnS}_2/\text{SnO}_2/\text{SSM}$ , they were acquired by partial hydrothermal phase while vulcanizing  $\text{SnO}_2/\text{SSM}$ . In general, 1.1 g of thioacetamide (0.5 M) was dissolved in DI water (30 ml) and treated to form a homogeneous precursor solution with magnetic stirring (30 min). Then the precursor solution and  $\text{SnO}_2/\text{SSM}$  mixture were moved to an autoclave of Teflon-lined

stainless steel and reacted (24 hours at 180°C). The SnS<sub>2</sub>/SnO<sub>2</sub>/SSM products were finally collected.

#### 4. Materials characterization

To have the morphology details of the items, scanning electron microscopy (SEM, FEI Verios 460) was used. Transmission electron microscopy (TEM, FEI Tecnai G2 F20 S-TWIN) equipped with energy-dispersive X-ray spectroscopy has identified the crystal structure of the samples (EDS). In order to gather the XRD patterns of the items, the D/max2200PC X-Ray diffractometer with CuK $\alpha$  radiation was used. photoelectron spectroscopy (XPS) instrument Axis Ultra X-ray. Was used to record the chemical state of elements was recorded.

#### 5. Electrochemical measurements

Electrochemical measurements by CR2032-type coin cells were performed by computer simulation to determine the potassium storage performance of the items. SnS<sub>2</sub>/SnO<sub>2</sub>-SSM was utilized as a working electrode to assemble the cells, and both counter and reference electrodes were used for the potassium metal. The mean mass load of active materials was determined before and after the hydrothermal reaction phase by measuring the weight of SSM substrate. The density of loading for active materials is approximately 1.2, and for SnO<sub>2</sub>/SSM, SnS<sub>2</sub>/SnO<sub>2</sub>/SSM, 1.0 mg cm<sup>-2</sup>. The electrolyte was a 1 M KPF<sub>6</sub> nonaqueous solution in a 1:1 (v/v) ethylene carbonate (EC) and diethyl carbonate mixture (DEC). Glass fiber (GF/D) from Whatman are the separators in this study. In a glove box packed with high-purity argon, the cells were assembled. The galvanostatic charge and discharge method was recorded at ambient temperature at various densities using the LAND-CT2011A device. The Cyclic Voltammetry (CV) curves were gained through an electrochemical workstation (CHI600E). A hydrothermal method was used to prepare the SnO<sub>2</sub> nanosheets/SSM materials. 1.2 g NaOH and 3.4 g SnCl<sub>2</sub>·2H<sub>2</sub>O (0.38 M) were dissolved in 40 mL ultrapure water at ambient temperature in a standard procedure to form a homogeneous precursor solution for 30 minutes under magnetic stirring. SSM was ultrasonically washed prior to being added to the above precursor in dilute hydrochloric acid, deionized water, ethanol and acetone, respectively. The mixture was then put in an autoclave of Teflon-lined stainless steel and heated in an oven for 24 h at 200°C and then naturally cooled at ambient temperature. SnO<sub>2</sub> nanosheets/SSM obtained were rinsed with ethanol ultrapure and water, then dried in the ambient atmosphere overnight at 80°C. SnO<sub>2</sub>/SSM samples with a SnCl<sub>2</sub> concentration of 0.2 M and 0.56 M have also been collected for comparison, although other conditions remain the same. On a D/max2200PC X-ray diffractometer with Cu K $\alpha$  radiation, X-ray diffraction (XRD) patterns were recorded. X-ray photoelectron spectroscopy was utilized to determine the surface chemical state of the elements (XPS, AXIS SUPRA). The CR2032-type coin cells were used to perform

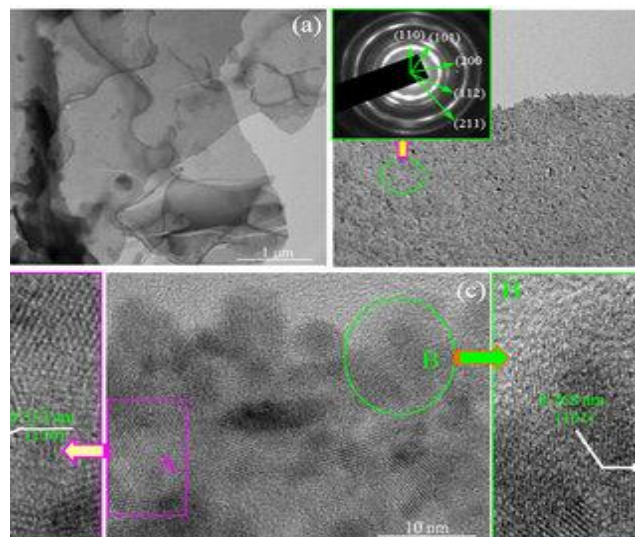


Fig. 6 SnO<sub>2</sub> Nano sheets, synthesis, characterization and structure

electrochemical measurements. The as-synthesized SnO<sub>2</sub>/SSM was the working electrode and the potassium metal acted as reference electrodes and the counter via simulation. Before and after SnO<sub>2</sub> was produced, the mass loading of SnO<sub>2</sub> was gained by weighing specific SSM substrates. On average, for SnO<sub>2</sub>/SSM-1, SnO<sub>2</sub>/SSM-2 and SnO<sub>2</sub>/SSM-3 the loading density of SnO<sub>2</sub> is 0.4, 1.6 and 3.8 mg cm<sup>-2</sup>. As an electrolyte, a 1 M KPF<sub>6</sub> nonaqueous solution was used in a 1:1 (v/v) mixture of ethylene carbonate (EC) and diethyl carbonate (DEC). Whatman's glass fiber (GF/D) was used as the dividers. They assembled and disassembled the coin cells in an argon-filled glove box. Using the LAND-CT2011A battery-testing instrument at ambient temperature, the coin cells were galvanostatically discharged and charged at various densities in a voltage span of 0.01-2.6 V. An electrochemistry workstation estimated CVs scanned at a voltage window of 0.01-2.5 V at 0.1 mV s<sup>-1</sup> (CHI618D).

#### 6. Result and discussion

The high and low magnification SEM images of SnO<sub>2</sub>/SSM samples was ready with various concentrations of SnCl<sub>2</sub> are illustrated in Fig. 8. From Figs.7(a)-(c), it could be shown that the metal wires were about 40  $\mu$ m in diameter. It was seen that as the concentration of SnCl<sub>2</sub> raised, the load of SnO<sub>2</sub> nanostructures slowly increased. Small Nano sheets less than 10 nm in size were grown on the SSM surface when the SnCl<sub>2</sub> concentration was 0.2 M, as shown in Fig. 7(d). Wide Nano sheets with a size of roughly 800 nm were collected on the SSM surface when the SnCl<sub>2</sub> concentration was increased to 0.38 M, as shown in Fig. 7(d).

It is possible to relate the formation of Nano sheets to the directed attachment of SnO<sub>2</sub> nanoparticles that shaped at the early phase of reactions. Because of more electrolyte contact area and short ion diffusion duration, these large

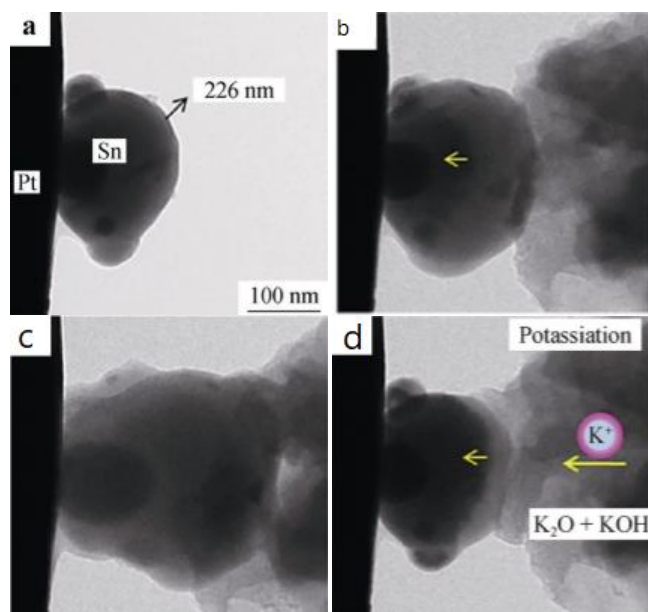


Fig. 7 (a) a pristine Sn nanoparticle; (b) first-step potassiation ion procedure, where arrows reflect path of  $K^+$  diffusion; (c) second-step potassiation ion process, without a definite boundary; (d) first-step potassiation ion process, where arrows show direction of  $K^+$  diffusion

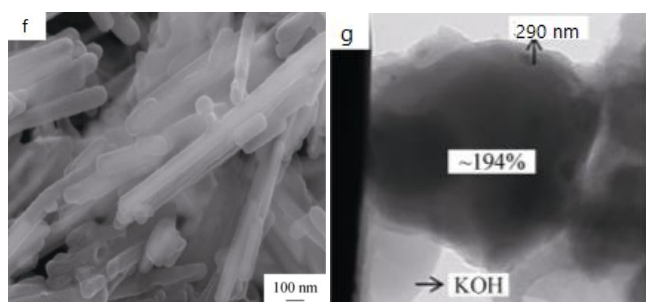


Fig. 8 SEM image and b TEM image; electrochemical performances of Sb@HCT as anode for PIBs: c cycling performance

size Nano sheets prefer high capacity in KIB electrodes. In Fig. 8(g), it can be shown that the film covered by large crystal particles on the surface of SSM increased to 0.48 M after the concentration of  $SnCl_2$ . As  $SnCl_2$  concentration raised from 0.2 M to 0.48 M, the morphologies of  $SnO_2$  changed from small Nano sheets by large Nano sheets to large crystal particles. The method of producing of the integrated  $SnS_2/SnO_2/SSM$  flexible binder-free electrodes is outlined in Fig. 7. Initially, by hydrothermal technique,  $SnO_2$  nano sheets were grown on SSM to obtain  $SnO_2/SSM$  (stage I). Subsequently, a hydrothermal vulcanization procedure through thioacetamide as a sulfur source (stage II) was performed on  $SnO_2/SSM$ . Finally, uniformly textured  $SnS_2/SnO_2$  hetero structured Nano sheets have been obtained on the SSM surface.

The  $SnO_2/SSM$  and  $SnS_2/SnO_2/SSM$  SEM images are shown in Figs. 7(a)-(d). The Nano sheets are ultra-thin with a grapheme-like morphology after the vulcanization process, as shown in Fig. 7(d). When tested as an alkali metal ion battery anode, the ultra-thin morphology can provide a large electrolyte interface area.  $SnO_2$  and

Table 1 Physical/electrochemical features and economic factors of lithium, sodium, and potassium

Physical/electrochemical properties/economic parameters	Li	Na	K
Atomic number	3	11	9
Atomic mass, u	6.941	22.989	39.098
Density, $g\ cm^{-3}$	0.535	0.968	0.856
Melting point, $^{\circ}C$	180.45	97.72	63.38
Atomic radius, pm	145	180	220
Ionic radius, $\text{\AA}$	0.76	1.02	1.38
Covalent radius, pm	128	166	203
Electronic shell structure	(1, 2)	(1, 2, 8)	(1, 2, 8)
Electronic configuration	(He) $2s^1$	(Ne) $3s^1$	(Ar) $4s^1$
Voltage vs SHE, V	-3.04	-2.71	-2.93
Theoretical capacity of the metal electrode, $mAh\ g^{-1}$	3861	1166	685
Crust abundance, mass %	0.0017	2.3	1.5
Crust abundance, molar %	0.005	2.1	0.78
Cost of carbonate, $US\$\ ton^{-1}$	6500	200	1000
Cost of industrial-grade metal, $US\$\ ton^{-1}$	100 000	3000	13 000

$SnS_2/SnO_2$ . TEM images are shown in Fig. 6. It is possible to see that  $SnS_2/SnO_2$  was seen as ultra-thin Nano sheets and rolled up some edges of  $SnS_2/SnO_2$  Nano sheets, further suggesting the graphene-like morphology. In Fig. 7(b), it can be seen that the mapping of  $SnS_2/SnO_2$  by energy-dispersive X-ray spectrometry (EDX) and the uniform distribution of Sn, O and S elements can be seen across the entire Nano layer. The  $SnS_2/SnO_2$  high-resolution transmission electron microscopy (HRTEM) image is shown in Fig 7(c). It is possible to align the crystalline fringes with space distances of 0.48 nm and 0.26 nm (Fig. 7(d)) with the (001)  $SnS_2$  and (101)  $SnO_2$  planes, respectively, suggesting that the partial  $SnO_2$  phase has been successfully converted to  $SnS_2$  phase. It is possible to clearly see the interface of  $SnS_2$  and  $SnO_2$ , as shown in Fig. 7(c), which is desirable for the movement of electrons along electrochemical reactions. Also, the phase compositions of the  $SnS_2/SnO_2/SSM$  products, XRD characterization was applied and the XRD pattern is illustrated in Fig. 8(f). The peaks diffracted at  $2\theta$  of  $43.6^{\circ}$  and  $50.8^{\circ}$  were indexed to SSM substrate. As shown in Fig. 8(g), new peaks were seen at  $2\theta$  of  $32.1^{\circ}$ ,  $41.8^{\circ}$  and  $49.9^{\circ}$ , which are well indexed with the (101), (102) and (110) planes of  $SnS_2$ . In order to acquire further knowledge about the chemical states on the  $SnS_2/SnO_2/SSM$  surface products, XPS was utilized. The standard range of an XPS survey in Fig. 8 demonstrates the existence of C, Sn, S and O, where the origin of element C is the adsorbed gaseous molecules. Using the elements composition presented in Table 1 which were extracted from XPS survey spectrum, the compositions of  $SnO_2$  and  $SnS_2$  are computed to be ca. 40 wt%  $SnO_2$  and 60 wt%  $SnS_2$

respectively. Figs. 7(b)-(d) shows the high resolution XPS spectra of Sn 3d, O 1s and S 2p. The peaks at 484.6 eV and 493.2 eV in Fig. 7(b) are adjusted to Sn 3d<sub>3/2</sub> and Sn 3d<sub>5/2</sub> peaks. The binding energy of O 1s in Fig. 7(c) is 532.2 eV, referring to Sn-O bonding's binding energy. The C-O and O-H bonds, which could be linked to the absorbed gaseous and H<sub>2</sub>O molecules, which can stem from the convoluted peaks at 533.9 and 530.0 eV. Via cyclic voltammetry (CV) and galvanostatic charge/discharge checking, the potassium storage properties of the SnS<sub>2</sub>/SnO<sub>2</sub>/SSM were assessed. Two pronounced cathodic peaks are observed at 0.64 and 1.51 V in the starting cycle for the SnS<sub>2</sub>/SnO<sub>2</sub>/SSM electrode relative to the CVs of the SnO<sub>2</sub>/SSM electrode, and then disappeared in the second and third cycles. The irreversible reactions and the presence of a stable solid-electrolyte interphase (SEI) film on the surface of SnS<sub>2</sub>/SnO<sub>2</sub> may be related to the inconsistency of CV curves. With almost complete overlapping, the subsequent cycles present strong reversibility, suggesting high reversibility during the reaction. The peak at 0.79 V can be assigned to forming the K<sub>x</sub>Sn alloys in the second cathodic scanning. While the peaks at 1.16 and 1.56 V may be due to the multistep de-alloying process of K<sub>x</sub>Sn in the second anodic scanning. The SnS<sub>2</sub>/SnO<sub>2</sub>/SSM electrode galvanostatic charge/discharge curves at 50 mA g<sup>-1</sup> are shown in Fig. 8(f). 722 mAh g<sup>-1</sup> and 474 mAh g<sup>-1</sup> are the discharge and charge capacities for the first cycle with a coulombic efficiency (CE) of 65.6%. Due to the reduced electrochemical resistance, SEI formation can play a critical part in obtaining a high CE after the initial cycle. The CE is, therefore, rising after the initial five cycles. For the 50th cycle, the charge and discharge power is 398 and 400 mAh g<sup>-1</sup> with a 99% higher CE. It can be seen that throughout the entire cycles, SnS<sub>2</sub>/SnO<sub>2</sub>/SSM tends to be greater than SnO<sub>2</sub>/SSM in terms of capacity. The discharge capacity of SnS<sub>2</sub>/SnO<sub>2</sub>/SSM can be maintained at 391 mAh g<sup>-1</sup> after 100 cycles, while the capacity of SnO<sub>2</sub>/SSM is 300 mAh g<sup>-1</sup>. On the basis of the 45 wt% SnO<sub>2</sub> and 50 wt% SnS<sub>2</sub> composition in the SnS<sub>2</sub>/SnO<sub>2</sub>/SSM, it can be inferred that SnS<sub>2</sub> and SnO<sub>2</sub> provide capacities of approximately 250 mAh g<sup>-1</sup> and 125 mAh g<sup>-1</sup>, respectively.

## 7. Conclusions

This study has focused on the economic and management use of rhododendron petals in potassium-ion Nano batteries anode via efficient Computer simulation. In this case, freestanding SnO<sub>2</sub>/SSM composites have been engineered and prepared as anode materials for PIBs. Freestanding SnO<sub>2</sub>/SSM composites were designed as anode materials for PIBs. They anchored the SnO<sub>2</sub> nanoparticles. Researches on performance improvement strategies and failure mechanisms of SnO<sub>2</sub> anode in full cell LIBs should be prioritized in order to realize the realistic application of SnO<sub>2</sub> in next generation LIBs with higher energy density, longer lifetime, higher protection, faster charge/discharge rate, and lower price. The low initial Coulombic efficiency is by far the most important concern of SnO<sub>2</sub> anodes in full cells (CE). Aside from low electrical conductivity, large volume expansion and slow reaction

kinetics, the key explanations for the seen degradation of reaction reversibility and power decay of SnO<sub>2</sub> are not as obvious as those of LIBs as anodes of SIBs and KIBs (i.e., coarsening of Sn NPs). The engineered synthesis of SnO<sub>2</sub>-based materials with optimal structures and components with high capacity and long life as anodes of SIBs and KIBs will direct the uncovering of these mechanisms. SnO<sub>2</sub>-based materials, however, have been thoroughly reviewed as anodes for batteries of Li-ion and Na-ion. Electrode technologies have been investigated to a reasonably mature stage for Li-ion batteries with recent material problems focusing primarily on protection, energy density and cost reduction by computer simulation. Electrode materials for Na-ion batteries are still under development, and electrode materials, particularly negative materials, should be further improved to meet the requirements for economically viable anode Na-ion batteries. In addition, various methods can boost the electrochemical efficiency of electrode materials, including growing electronic conductivity, shrinking the duration of ion diffusion, changing microstructures, and compositing with carbonaceous materials.

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