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Workshop on Electrochemical Energy Storage: Theory, Experiments, and Applications | (SMR 3698)

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P01

Efficient synthesis of enwrapped CuO@rGO nanowire arrays to improve supercapacitor electrode performance

There has been a growing interest in the performance of supercapacitors (SCs) based on Transition Metal Oxides (TMOs). It has recently been included in long-term energy storage and lightweight devices. The primary goal of this research is to improve the conductivity of CuO nanowire to increase its performance. We have successfully synthesized a wet chemical utilizing a dipping approach in this paper. rGO nanosheet layers were uniformly coated on CuO nanowire arrays. As long as positive, stable pathways for rapid ion or electron transport exist, the presence of atoms in rGO that will diffuse into the CuO lattice may improve the electrical conductivity of the CuO electrode. Furthermore, the surface area of the CuO@rGO-20 s electrode was also increased following rGO coating, resulting in more active sites. As a result, CuO@rGO-20 s electrode had a significantly greater areal capacitance of 1165 mF cm^{-2}, which was 2.4 times higher than pristine CuO NWAs and excellent extended cycling performance 119% after 2000 cycles as a pseudocapacitive electrode. Overall, our data indicate that enhancing TMOs electrode performance has a considerable impact. Graphical abstract

P02

Proton interacalation batteries

energy storage devices are the burning topics of research for todays world which demands portable energy storage devices. Various research works in the differents parts of the world is been focusing on this topics . With the insurgence of Lithium ion batteries, the energy field is boosted in a new direction. But there are some shortcomings of lithium ion batteries, like availability crisis, cost, eco friendliness etc. So to overcome this difficulties and to get a new system various attempts are performed by the research communities.Sodium ion batteries, aluminium ion batteries, potassium ion batteries are some of the best examples which in near future will boast ours energy storage system.Motivated by this we also try a very common system of proton intercalation as a energy storage system.Our work is done on aqueous environment, with all the necessary points to be satisfied as ecofriendly energy storage system. This priliminary work will definitely going to boast the thriving energy requirements of the present world in near future.

P03

Nanoparticles/Thermotropic Liquid Crystal Nanocomposites Phase Changing Materials for the Development of Storage Applications

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Abstract

Liquid crystals composites have many promising application which motivate us to undertake non-volatile memory effect for the electronic storage devices [1-2]. In this perspective, we fabricate memory devices with different nanoparticles (aerosil and CdS) doped into thermotropic liquid crystal (KCFLC 10r). To investigate the non-volatile memory, the dielectric spectroscopy, optical microscopy and electro-optical response techniques have been performed. The obtained experimental results emphasizes the prominence of guest nanoparticles in pure LC, which lead to retrieve a long lasting memory in doped devices. The achieved prolonged memory effect in doped samples is due to induced charge transfer near the surface under the application of applied field. This mechanism responsible for ion trapping effect result in minimization of depolarized field and memory effect in doped samples. Hence, such systems may be helpful to design as low power, non-volatile electro-optical memory devices for innovative information storage applications.

Keywords: Thermotropic liquid crystal; nanoparticles; memory effect

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P04

Adsorption of Alkali Metal Ion on Basal Functionalized Graphene: A study from DFT

The importance of a battery's first charge-discharge cycle relates to the irreversible capacity loss due to the reaction of the alkaline metallic ions. In graphenic materials, this loss is related to the presence of oxygenated functional groups present in the material. The present work uses computational methods to study the interaction between the ions and these functional groups located in the basal plane of the graphene. Additionally, the influence of these anions on the battery performance is also evaluated from an electrochemical perspective to determine the performance of alkali-ion batteries based on graphenic anodes.

P05

Cobalt-Phosphide encapsulated with Nitrogen-rich Carbon nano framework for high performance All Solid-State Lithium ion batteries

Employability of solid state electrolyte in Lithium ion batteries can successfully circumvent issues of leakages and explosion associated with presence of organic liquid electrolytes while simultaneously promising better energy density due to provision for short length diffusion pathways for ions. While on another aspect, despite having high theoretical capacity and lower redox potential, lithium storage performance of Phosphides as anode is hindered due to volume alterations and conductivity on lower side. Herein, Cobalt phosphides nanoparticles encapsulated with nitrogen-rich carbon framework are synthesized using ZIF-67 based sacrificial template that showed superior electrochemical performance as an anode material for All solid-state lithium-ion batteries (ASSLIBs).Charge storing mechanism for hierarchical Co2P have been established using XRD. The in situ generated carbon framework act as a porous network with Co2P nanoparticles uniformly embedded in nitrogen-doped carbon skeleton provided superior lithium storage performance. Co2P@NCF could deliver high initial charging and discharging capacities of 1335.9 and 1284.7 mAh g-1 at a 0.1C rate with coulombic efficiency of above 100% till 30th cycle. Further the electrode could withstand strains due to cycling as evident from its superior cycling performance. Benefitting from hierarchical structural features, the Co2P@NCF electrode is demonstrated to be promising as an anode for ASSLIBs.

P06

Computational studies on electrochemical performances of doped and substituted $Ti_3C_2O_2$ MXene

Using Density functional theory (DFT) in conjunction with a solvation model we have investigated the phenomenon of eletrode- electrolyte interaction at the electrode surface and its consequences on the electrochemical properties like the charge storage and total capacitance of doped and substituted oxygen functionalised Ti_3C_2 supercapcitor electrode. We have studied nitrogen doped, nitrogen sub- stituted and molybdenum substituted Mxenes in acidic electrolyte H_2SO_4 solution. By considering nitrogen doping at different sites, we found that the greatest capacitance is obtained for doping at functional sites. Our results agree well with the available experiment. We also found that the en- hancement in capacitances due to nitrogen doping is due to amplifications in the pseudocapcitances. We propose that the primary mechanism leading to the enhanced value of the capacitances due to nitrogen doping is surface redox activity. The performances for substituted systems, on the other hand, are degraded in comparison to the pristine ones. This suggests that better storage capacities in $Ti_3C_2O_2$ electrode can be obtained by doping only. We provide insights into the reasons behind contrasting behaviour in doped and substituted systems and suggest ways to further improve the capacitances in doped system.

P07

SIB's over LIB's

Sodium-ion batteries (SIBs) are currently evolving as a viable substitute for lithium-ion batteries (LIBs) because of the abundant availability and reasonable cost of sodium. As Na is thrice heavier and possesses a lower standard electrochemical potential than Li, it makes the built-in SIBs difficult to outclass the LIBs in terms of energy density, specific capacity, or rate capability. In SIBs, thus far investigation of cathode materials such as poly anionic compounds and layered transition metal oxides has been the center of attention in the ongoing research and very limited emphasis is paid to anodes materials. Generally, assessment of SIB anode materials needs an adequate correlation with the analogue reaction in LIBs. Hence, recent researches are directed toward the advancement of worthy anode materials for SIBs, which can enable the overall reactions at large energy densities with reasonable cost. In the same vein, metal sulfides and their composites with carbon have lately attracted a good deal of attention as high-performance anode to the development of SIBs. Therefore, in this chapter we have systematically discussed the different reaction mechanisms and accounted the development of metal sulfide–based materials and their challenges in SIB anodes.

A high-performing Sulfur-based electrolyte for Lithium-Sulfur batteries: a first-principles study

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Abstract

Recently, there has been significant interest in developing solid-state electrolytes (SSE) for lithium-ion batteries and related technologies. Using first-principles calculations based on density functional theory (DFT) and the nudged elastic band (NEB) method, we have reported an investigation on the optimized crystalline structure of β-Li_3PS_4; an idealized crystal phase of the electrolyte "Lithium thiophosphate Li_3PS_4". We examined its electronic properties through band structure and density of state calculations where we found that our calculated bandgap energy is consistent with the one reported in the literature from first-principles calculations. In addition, we have examined in this study the possible Li-ion diffusion pathways within β-Li_3PS_4, the Li-ion diffusion barrier energies and ionic conductivity of the system. Furthermore, we will investigate the improved ionic conduction and activation barrier as a function of the increased site disorders resulting from the effect of doping.

These calculations will further help guide our experiments to deliver the best-performing SSE materials with the ideal composition.

Keywords: Lithium-Sulfur Batteries, Li-ion Diffusion, Li_3PS_4, Density Functional Theory.

Applications of XPS simulations in the Characterization of Solid Electrolyte Interphase in Li-ion Batteries

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During the operation of lithium-ion batteries (LIBs), a solid electrolyte interphase (SEI) layer forms on the graphite surface, due to side reactions with the electrolyte solvent and salt. While the SEI layer can prevent the exfoliation of graphite materials and inhibit further electrolyte decomposition, it has an impact on its initial capacity loss, self-discharge characteristics, cycle life, rate capability and safety. Therefore, investigation of the dynamic evolution and spatial composition of the SEI film in the organic electrolytes can aim toward improving the electrochemical performance and the formation cycles of lithium-ion batteries (LIB). Different chemical analysis technics such as X-ray photoemission spectroscopy (XPS) and X-ray absorption spectroscopy (XAS) methods can be used to analyze the chemical-phase composition and the interfacial processes, between electrode and electrolyte. However, regarding the complexity of SEI structures, interpretation of the experimental data is extremely difficult. The assignments of experimental XPS and XAS signals are normally based on references obtained from molecular or crystalline samples, which are simplified approximations for the far more complex structures. Here, we design a workflow to calculate the XAS and XPS signatures of the simulated SEI structures in more realistic environments, building a dataset that can be used for deconvolution of experimental spectra as well as providing the depth-profile spectra. Our SEI structure was simulated by using the kinetic approach to the Monte Carlo-molecular dynamics (MC-MD) method [1].

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P10

Flow induced vibration-based energy harvesting under two aerodynamic forces

This paper examines galloping-based piezoelectric energy harvesting (GPEH) in a linear two-degree-of-freedom (2-DOF) mechanical system that is coupled to an electrical circuit through a piezoelectric mechanism. For the current investigation, A 2-DOF galloping-based piezoelectric energy harvester by mounting a primary piezoelectric system on a secondary system under two aerodynamic forces, one force for every mass. For comparative analysis between two configurations, we investigate the case of the primary system is only excited by the aerodynamic force compared to the point of the primary and secondary system are both excited by the aerodynamic force. The complexification-averaging (CX-A) method is applied to obtain approximate solutions. The analytically observed responses is numerically explained. In order to establish the feasibility of the proposed method, the energy balance of system is investigated. Our findings demonstrate that the combination of two aerodynamic forces enables the system to harvest high periodic power output compared to the conventional 2-DOF GPEH system with a single hydrodynamic force. Also, a good galloping energy harvester is expected to have a low critical wind galloping speed and a high power output.

P11

New Trending Polymer Based 2D Nano Structure Material for Storage Devices and Sensing Applications

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Abstract:

A new polymer based 2D nano structured material with various morphologies such as hybrid core-shell, nano tube, nano fibres, cubic, hexagonal, and flower structured materials are emerging new trends advanced multifunctional characteristics due to its novel chemical/physical properties including their size, shape, good electrical conductivity, electrochemical performance, optical properties, photoluminescence, abundant edge defects, and better photovoltaic properties making them most prominent candidature for various energy storage, conversion, and sensing devices. Synthesized the conjugate polymer based 2D materials with different nano structured by using facile synthesis methods at different environmental conditions and different strategy. Characterisations of nano structured material will be done with help of characterised techniques and confirmed the proper dispersion as well as morphology. The storage capacity and sensitivity characteristics are evaluated and obtained results suggesting that these new trending nano structured materials could be creating new dimension in the storage capacity and sensing applications. Thus, high specific capacitance and good stability of nanocomposite encouraging the promising application in high performance energy storage devices.

P12

Ab-initio Study of Lithium Intercalation into a Graphite Nanoparticle

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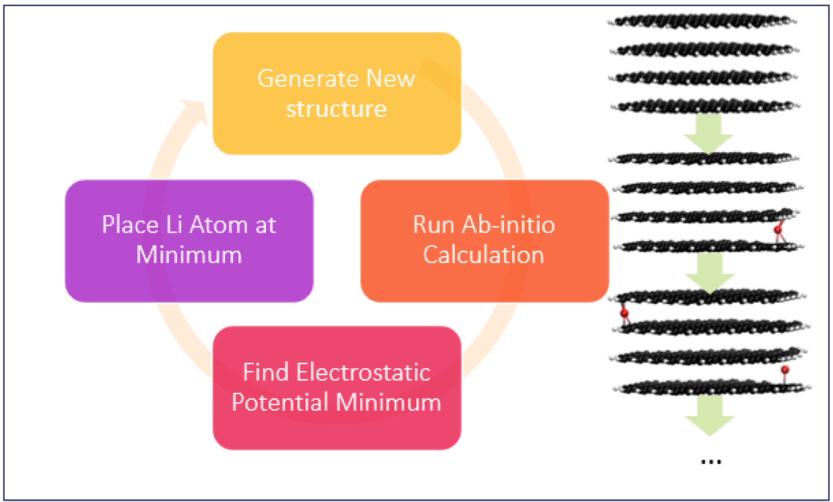
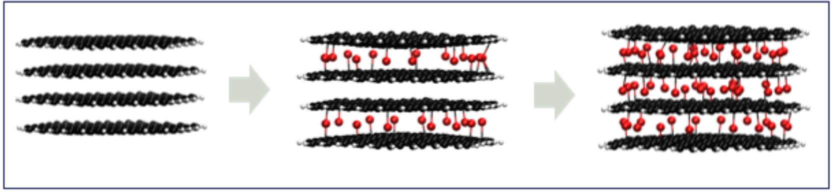
The process of Li intercalation in electrodes is fundamental to the operation of Li-ion batteries. The computational modelling of this process at atomic resolution will contribute greatly to the rational design of improved battery materials. Towards this goal, we present an approach and workflow for the simulation of Li intercalation which uses electrostatic considerations. These considerations use the electrostatic potential found from Density Functional Theory (DFT) calculations as a guiding principle to locate favourable sites for Li intercalation. We test the method on a material representing an anode-like structure, graphite nanoparticles. The study of nanoparticles using first-principles methods is made available to us through linear-scaling DFT program, ONETEP[1], which allows calculations on larger numbers of atoms than conventional DFT. We show how our approach can reproduce the well-known Li staging, and we investigate the electronic structure of the nanoparticle obtained via atomic charges and density of states analysis. We also compute the voltage step profiles of the structures via a convex hull formalism and find reasonable agreement with experimental open circuit voltages with respect to the degree of Li intercalation. Our approach provides a novel route to simulating the intercalation process and, combined with linear-scaling DFT, can be used to investigate intercalation in complex nanoscale electrode structures.





(1) Prentice et al. The ONETEP Linear-Scaling Density Functional Theory Program. *J. Chem. Phys.* **2020**, *152* (17), 174111. https://doi.org/10.1063/5.0004445.

Hydrogen storage properties of MgH_2 alloys produced by high energy ball milling

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Introduction:

Regarding the use of hydrogen in fuel cell for mobile or stationary applications, metal hydrides can offer a high hydrogen volume capacity and a safe alternative compared with liquid storage or with compressed gas. Among the metal hydrides, magnesium is considered as one of potential hydrogen storage materials because of its high capacity (7.6 wt%), lightweight and low cost. However, high work temperature, slow reaction kinetics and hard activation process limit the practical application of Mg-based hydrides. Recently, the reactive ball milling was successfully introduced to prepare hydrogen storage materials. In this work, MgH_2 catalyzed with Ni nanoparticle was synthesized by high pressure reactive milling under hydrogen up to 100 bar.

Experimental:

MgH2 (Goldschmidt, 95+%), Ni (99.9%, Sigma Aldrich, ~90 nm) powders were used. The powders were filled into a hardened steel vial and sealed together with 13 balls (9.5 mm in diameter) and reactively milled in a planetary mill Fritsch (P6) at a rotational speed of 400 rpm (ball to powder ratio 10:1) for 2 hours under hydrogen (0-100 bar) atmosphere. Structural changes during milling were characterised by XRD (Co-K_α) and high resolution scanning electron microscopy. Hydrogen sorption properties have been studied by gravimetric analysis in a wide temperature and pressure range for absorption (1-10 bar, 50-300 °C) and desorption (250-350 °C, 50 mbar-1 bar). Thermal properties of samples were studied using a differential scanning calorimeter (DSC, Netsch) with H_2 flow rate of 10 K/min.

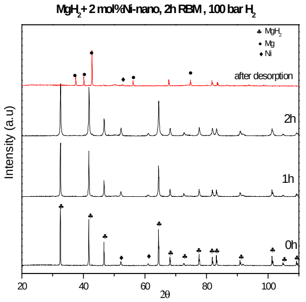


Figure 1: X-ray diffraction patterns of MgH2-2mol%Ni nanoparticle produced via reactive ball milling for 2 hours and after H2 absorption/desorption cycling, ended with desorption at 350 °C, 50 mbar.

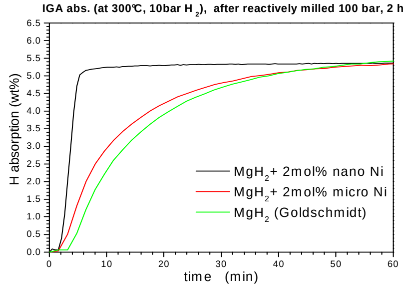
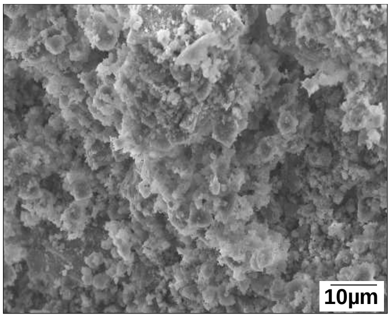


Figure 2: Hydrogen absorption of MgH2-2mol% Ni nanoparticles compare to microparticles and pure MgH2 samples at constant temperatures and pressures after reactive milling under 100 bar H2 for 2 hours.



SEM image of MgH2-2 mol% Ni nanoparticle after high pressure reactive milling for 2 h

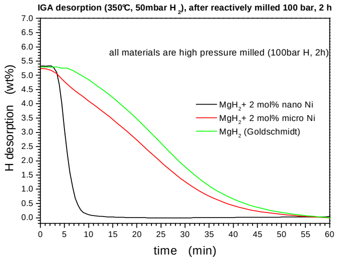


Figure 3: Hydrogen desorption of MgH2-2mol% Ni nanoparticles compare to microparticles and pure MgH2 samples at constant temperatures and pressures after reactive milling under 100 bar H2 for 2 hours.

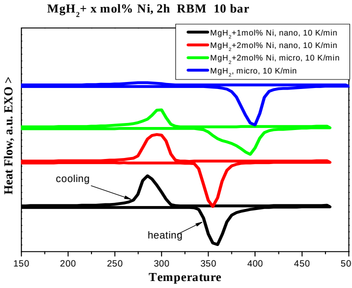
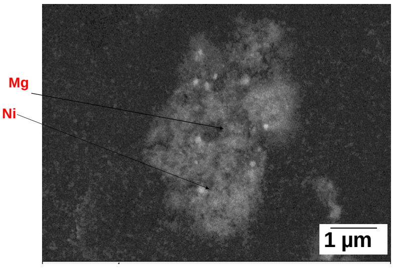


Figure 4. DSC thermodynamic investigation of MgH_2 catalyzed with varous type of Ni and compared to pure MgH_2. H2 flow rate of 10 K/min.



BSE image after desorption showing the presence of Mg and Ni (white spot), which is dispersed on the surface of Mg

Summary:

- High hydrogen absorption / desorption kinetics, which are stable upon cycling and far superior to nanocrystalline magnesium hydride are observed.
- Absorption conditions have been found to be quite modest at 300 °C and 5.5 wt.% is reached within 5 min. Desorption into 1 bar hydrogen can be achieved at 350°C within a few minutes.
- MgH2 catalyzed with small amount of nickel nanoparticles prepared via high pressure reactively milling has been done. This process results in high surface area powders with finely dispersed Ni- particles on the surface of Mg.
- The metallic Ni in nanometer scale acts as a catalyst for improvement the kinetics of MgH2 for hydrogen storage material and at the same time allowed to reduce the milling process for short time, only 2 hours.
- As expected, no changes in thermodynamic properties (DSC result) were observed

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P14

Fabrication and Characterization of Banana (Musa acuminata) Cotton Blended Textile with Multi-walled Carbon Nanotubes and Polypyrrole as Supercapacitor Electrode Materials

The recent advancements of technology in our society and the exponential growth of human population has led to higher consumption and necessity for energy. Fossil fuels and other renewable energies are essential in fulfilling our energy demands, but they lack the capacity for its storage. Driven by this demand for energy storage, researchers are pushing to develop electrical energy storage devices such as supercapacitors to solve these problems. The objective of this study is to fabricate and characterize banana-cotton fabric (BCF) with multiwalled carbon nanotubes (MWCNT) and polypyrrole (PPy) as electrode materials for flexible supercapacitors. The pristine BCF coated with MWCNT via dip-and-dry method gave a loading of 0.5 mg/cm2. Then PPy coating was completed via in situ chemical polymerization. Using the four-point probe conductivity probe, these composites showed conductivity values for MWCNT/BCF of 2.18 x 10-2 S/cm (64.2 % RSD, n=3), for PPy/BCF: 3.92 x 10-2 S/cm (22.3 % RSD, n=3), and for PPy/MWCNT/BCF: 2.86 x 10-1 S/cm (67.3 % RSD, n=3). The composite electrodes were electrochemically characterized using cyclic voltammetry. These are the areal capacitance values exhibited by the following composites: 7.29 mF/cm2 (42.5 % RSD, n=3) for MWCNT/BCF, 2.12 x 102 mF/cm2 (27.6 % RSD, n=3) for PPy/BCF, and 4.53 x 102 mF/cm2 (71.2 % RSD, n=3) for PPy/MWCNT/BCF. These results showed that PPy/MWCNT/BCF produced the highest conductivity and areal capacitance value which can be attributed to the combined electrochemical properties of MWCNT and PPy. The electrodes were further characterized using scanning electron microscopy (SEM) for the morphology, Fourier transform infrared spectroscopy (FTIR) for the chemical structure, and thermogravimetric analysis (TGA) for the thermal stability. Furthermore, additional electrochemical characterizations like electrochemical impedance spectroscopy (EIS) had shown minimal solution and charge transfer resistance values of 0.56 Ω and 2.7 Ω, respectively. The supercapacitor fabric electrode registered a galvanostatic charge-discharge (GCD) of 311 W/kg for the and 7.51 Wh/kg for power density and energy density for the full cell, and cycling stability of 33.4% decay after 500 cycles.
Keywords: polypyrrole, multi-walled carbon nanotubes, fabric supercapacitors

P15

Feasibility of Anions for Developing New Water-in-Salt Electrolytes for Lithium-Ion Batteries: A DFT study

Electrolytes are an essential component for assuring the security, performance, and cycle life of a battery. An alternative to the current commercial organic electrolytes are aqueous electrolytes. This type of electrolyte is characterized by having a narrow electrochemical stability window; however, this can be extended by increasing the concentration of lithium salts (water-in-salt) as the electrolyte stability relies on the anion. In this work, the stability of these anions with respect to their reduction (cathode) and oxidation (anode) was evaluated using computational methods, rationalizing the usage possibilities of lithium salts with inorganic (common salts), fluorinated, and carboxylated anions. Finally, through these methods is also possible to predict the species that might form on the SEI (anode) and CEI (cathode).

P16

The Li_xSi_y class of compounds exhibits a broad variety of crystal structures depending on the exact stoichiometry, with surprising differences in lithium diffusivity. We perform a systematic series of *ab initio* molecular dynamics simulations in order to characterize the mobility of lithium atoms, both from a local and from a long-range perspective. Our study shows the crucial importance of including interstitial sites in description of diffusion. Since the diffusive behavior of lithium in these compounds can be attributed to recurring diffusion paths, we identify pathways in our simulation trajectories and further investigate them by means of nudged elastic band calculations to obtain energy profiles. We show the connection between diffusion mechanisms and migration energy barriers and especially highlight the relevance of point defects for low migration energies. Furthermore, we study the influence of the motion of lithium and silicon atoms that are adjacent to diffusing lithium atoms along their paths and draw special attention to the importance of this motion for energetic stabilization of self-interstitial lithium atoms.

P17

Novel cobalt phthalocyanine as dual catalyst for oxygen reduction reaction and air cathode battery

The synthesis of novel tetra 4-{[5-methyl-2-(propan-2-yl) cyclohexyl] oxy} cobalt phthalocyanine (TmCoPc) is described for the first time in this study. The novel synthesized TmCoPc was characterized by UV-Vis, FTIR, XRD, HRMS, 1H NMR, and TGA. The synthesized non-precious electrocatalyst TmCoPc /super-p (or TmCoPc /SP) was used as Ptfree electrocatalyst for the effective oxygen reduction reaction (ORR) in order to overcome the sluggish cathode kinetics of ORR on bench mark electrocatalyst Pt/C which has severely postponed the commercialization of PEM fuel cells. Pt-free non-precious electrocatalyst TmCoPc /SP catalyst exhibited sluggish-free with excellent activity for ORR. The RRDE analysis showed that the ORR undergoes a two-step pathway on the basis of the calculated number of electrons transferred (n) per oxygen molecule and the proportion of peroxide species (% H2O2) generated during the ORR. Further, in metal-air batteries and fuel cells, the electrons are captured by oxygen atoms having positive redox energy. Further, here a battery concept is demonstrated, wherein the electrons emitted by the anode are driven to cause a oxygen reduction reaction and therefore, the cathode function as an air reactor. The battery supplied 1.41 V open-circuit voltage, a maximum peak power density of 72 mW/cm2 at 123mA/ cm2 maximum peak current output. The oxygen reduction reaction discharged only water as byproduct.

P18

3D printing of pristine graphene ink and graphene quantum dots and their electrochemistry

Due to its capacity to manufacture low-cost 3D-printed structures, 3D-printing technology offers a unique opportunity for the fast epitome of various applications. Using a typical fused deposition modeling 3D printer along with a Discovery extruder, a graphene-ink can be 3D printed to produce an interdigitated electrode (IDE) arrangement. This work fabricated a 3D-printed planar supercapacitor from pristine graphene-ink without using high-temperature processing or functional additives. The printable ink (89%) is formulated from pristine graphene without the addition of any functional additives. The symmetric flexible supercapacitor is demonstrated with an excellent specific capacitance of 137.50 F/g at 0.5 A/g and an energy density of 12.23 Wh/kg. The obtained gravimetric energy density beats reported earlier carbon-based supercapacitors that are 3D or inkjet printed. The flexibility and robustness of 3D-printed devices are achieved up to 150° folding angles. This work demonstrates an efficient and easy method for fabricating practical energy storage devices featuring a customizable shape and excellent flexibility.

P19

Theoretical Investigation of Substitutional doping of Transition Metal in MoS_2 for Enhanced Electrocatalytic Hydrogen Evolution Reaction

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Abstract

Extremely active, abundant and low-cost electrochemical catalysts for reactions such as the Hydrogen Evolution Reaction (HER) are essential for the development of efficient electrode material as well as for effective water-splitting techniques. The study of multilayer TMDCs, particularly those of Molybdenum Disulfides (MoS_2), has become great interest for material scientists for its application encompassing topics like energy storage, catalysis, and others. When compared to pure MoS_2, doping TMDCs with transition metals such as (Ni, Co, Nb, Re) can improve their performance in HER applications and hence expand their good prospect. To study the detailed HER mechanism, hydrogen adsorbed over different sites like Mo-edge, S-edge, bridge (on the bond), and center of hexagon etc, subsequently symbolizing to be HER active. All simulations were executed using first-principle calculations based on Density Functional Theory (DFT) using Quantum Espresso package. As theoretical simulations have proven to be effective in revealing the links between the electronic structure of materials and their catalytic activity, and hence in addressing for forecasting and developing better catalysts. The catalytic activity is due to the optimal electron transfer from a transition metal to MoS_2. This electron transfer facilitates H^* interaction and adsorption, leading to reduction in Gibb's free energy and local work function, which hence intensifies the HER performances. Ultimately, the possibility of modifying active sites in MoS_2 through an appropriate /pertinent choice of metal dopants opens up further opportunities for selectively improving the catalytic behavior of this material.

P20

Surface structure decoration of high capacity Li1.2Mn0.54Ni0.13Co0.13O2 cathode by mixed conductive coating Un-zipped MWCNTs for lithium-ion batteries

Multiply depolarized composite cathode consisting Li1.2Mn0.54Ni0.13Co0.13O2 (LMNCO) and un-zipped multi-wall carbon nanotubes (UZ-MWCNTs) is prepared via pasting LMNCO/UZ-MWCNTs composite slurry on Al foil. Where, UZ-MWCNTs consist of a conductive network of graphene nano-ribbon (GNR) and carbon nanotubes (CNTs). The concentration of UN-MWCNTs was varied to see its effects on the performance of cathode. The interlocked conductive network of GNR and CNTs stabilizes the structure of composite and also improves Li ion transport and the electronic conductivity.

P21

Applicability of bioploymer based composite in electrochemical energy storage

Starch based ternary composites (Starch/rGO/MoS_2) synthesized by chemical reduction, hydrothermal method accordingly. Then the film is prepared by the addition of raw material with plasticizer. The nanostructure of starch/rGO/MoS_2 is confirmed by XRD, FTIR, and SEM analysis. The starch/rGO/MoS_2 (1%) composite exhibits the highest specific capacitance (124 F g^{-1}) and cycling stabilities (100% retain capacitance after 1000 cycles). The excellent electrochemical capacitive performance is attributed to its 3D network structure and the synergistic effects among the three components that make the composites obtain both pseudo capacitance and double-layer capacitance.

P22

Study of magnetic, and electronic of $LiVOPO_4$ cathode

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Abstract:

We have used the self-consistent *ab initio* calculations, based on Density Functional Theory approach and using Full potential Linear Augmented Plane Wave (FLAPW) method, high temperature series expansions calculations and Monte Carlo simulation to study the electronic magnetic and properties of $LiVOPO_4$, and $VOPO_4$ compounds. The average equilibrium voltage over a full cycle (V_{cell}) of the $LiVOPO_4$, battery is estimated from our FLAPW calculations. Computed magnetic moments are used as input for the high temperature series expansions calculations (HTSEs) to compute other magnetic parameters of two compounds. We have deduced the first and second exchange interactions between the magnetic atoms V-V in $LiVOPO_4$ using the mean field theory. The Monte Carlo simulations (MCSs) is used to study the magnetic properties of $LiVOPO_4$.

P23

Raman Spectroscopy Technique as an Effective Tool to Monitor Dilution Effects on Ionic Liquids

Ionic liquids (ILs) properties are very flexible as a function of addition of water or other solvents. This property makes them interesting candidates as solvation media to assess the stability and structural changes of dissolved biomolecules. Yet, the molecular structure of the mixtures itself needs to be understood. In this work four imidazolium based ionic liquids (1 methylimidazolium Cl, 1 methylimidazolium tfo, 1 methylimidazolium NO_3, 1 methylimidazolium HSO_4) have been studied by Raman spectroscopy using two excitation wavelengths, one in the UV range (266 nm) and the other in NIR range (785 nm). Most of the imidazolium cation bands show intensity enhancement at UV excitation as a result of the phenomenon of pre resonance. Specific spectral differences among the different samples were identified, at high and moderate IL concentrations, attributed to changes on cation anion interactions. In a highly diluted samples (water ratio > 90%) all samples tend to have more similar spectra, suggesting analogous hydration features of the cation in these conditions. The results from the present Raman investigation contribute to a more comprehensive view of the water mediated interactions in IL/water mixtures. This could facilitate the design of effective stabilizing ILs for their exploitation in the fields of biomedicine and life science

P24

Black phosphorene/blue phosphorene van der Waals heterostructure: a potential anode material for lithium-ion batteries†

Van der Waals (vdW) heterostructure-based electrodes have invoked tremendous research interest due to their intriguing properties and their capability to break the limitations of the restricted properties of single-material systems. Herein, based on first-principles approaches, we propose that the black phosphorene/blue phosphorene (BLK-P/BLE-P) vdW heterostructure can be a capable anode material for power-driving lithium-ion batteries (LIBs), as it exhibits a large theoretical capacity, together with a relatively strong binding strength compared with the individual BLK-P and BLE-P monolayers. Our calculation results show that the Li adatom prefers to intercalate into the interlayer of the BLK-P/BLE-P vdW heterostructure due to the synergistic interfacial effect, resulting in high binding strength and a diffusivity comparable to the BLK-P and BLE-P monolayers. Subsequently, the theoretical specific capacity is found to be as high as 552.8 mA h g-1, which can be attributed to the much higher storage capacity of Li adatoms in the BLK-P/BLE-P vdW heterostructure. Furthermore, electronic structure calculations reveal that a large amount of charge transfer assists in semiconductor to metallic transition upon lithiation, which would ensure good electrical conductivity. These simulations prove that the BLK-P/BLE-P heterostructure has great potential in LIBs and is essential for future battery design.

Structural and electronic properties of $Li_4Ti_5O_{12}$ and G/ $Li_4Ti_5O_{12}$(111) composite materials: A first principles study

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We have studied the structural and electronic properties of bulk $Li_4Ti_5O_{12}$ (LTO) and G/LTO(111) composite materials, as an anode material for lithium-ion batteries using the first-principles method, as implemented by the VASP code. We have shown that the bulk LTO material exhibits insulating behavior with the bandgap of 2.94 and 3.6 eV using the GGA and GGA+U calculations respectively. The diffusion pathways are optimized and the energy barriers of lithium migration along the pathways are calculated with the nudged elastic band method (NEB). Our results show that the lithium diffusion in the charged state energy barrier is 0.2 eV respectively. In addition, we investigated the interfacial electronic structure, charge transfer properties and formation energy of graphene physisorption and chemisorption on the various different LTO(111) surfaces (Oxygen, Lithium, Titanium, Lithium and Titanium terminated surfaces) from calculations. Our calculations is indicated to show a chemisorption property for Oxygen terminated surfaces (G/LTO$(111)_{O}$) and a physisorption property for other surfaces (G/LTO$(111)_{Li}$, G/LTO$(111)_{Ti}$, G/LTO$(111)_{Ti,Li}$). Hence, our calculations show that a slight charge transfer occurs in the physisorption case while a significant charge transfer takes place in the chemisorption configuration. In finally we have shown that the most stable structures for calculating formation energy were surfaces with G/LTO$(111)_{Li}$.

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P26

Binder Free Paper based Electrodes for Hydrogen Evolution and Supercapacitor Applications

Liquid phase exfoliated transition metal dichlcogenides have been considered as promising electrode materials for high performance electrocatalysts for water splitting and pseudocapacitors because they offer higher electrochemical activity than the bulk crystals owing to high concentration of edge active sites. The system model of binder-free electrode architecture is an expedient approach for enhancing the endurance of electrochemical supercapacitors. Herein, we report the flexible, large area and robust paper-based electrode functionalised by electrochemically active 1T-rehenium disulphide (ReS2) nanocrystals. 1T-ReS2 nanocrystals on cellulose paper electrode was used as binder free electrode that exhibits the low over potential of 170 mV and stable charge transport for 14 hours. Extremely low series resistance of 2 Ω and charge transfer resistance of 5 Ω are achieved for electrically and electrochemically conducting electrodes. Paper based electrode also exhibits high specific capacitance of 120.8 F g-1 at scan rate of 5 mV s-1 and 153.2 F g-1 at 1 A g-1. Encouragingly, electrode demonstrate the 100% retention of capacitance after 1000 cycles with advantage of being light weight. This research paves the foundation for the expansion of large-scale active catalysts using an intrinsic charge engineering approach.

P27

MODELLING THE ELECTRODE CALENDERING PROCESSES OF LITHIUM ION BATTERIES (LIB)

There has been a recent increase in the demand for high-performing and durable Li-ion batteries (LIBs) for renewable energy storage. This has necessitated the use of optimization techniques in the manufacturing process. Calendering is one of the critical processes that influence the electrochemical and physicochemical interactions (AM, CBD, porosity, pressure, and thickness). These processes are highly complex, making them very time-consuming and resource-intensive. Data acquired for (NMC) based cathodes were generated from an in-house stochastic electrode mesostructure by the Artistic Project. A data-driven approach (support vector regression (SVR)) was used to develop models to predict the mesoscale electrode properties of the LIB. The models were trained and tested on the acquired data. Their predictive accuracy results were; liquid-phase tortuosity - 74%, solid-phase tortuosity - 73%, the percentage of CC/AM - 51%, the percentage of CC/CBD - 75%, active surface - 71%, porosity after calendering - 72% and the effective conductivity - 72%. The predictive ability of the models shows that it is capable of optimizing the time and resources used during the manufacturing process of the battery and can also predict the influence of the calendering process on the final NMCs electrode properties, as this would help future manufacturing processes.

P28

Graphene for rechargeable non-aqueous aluminum battery

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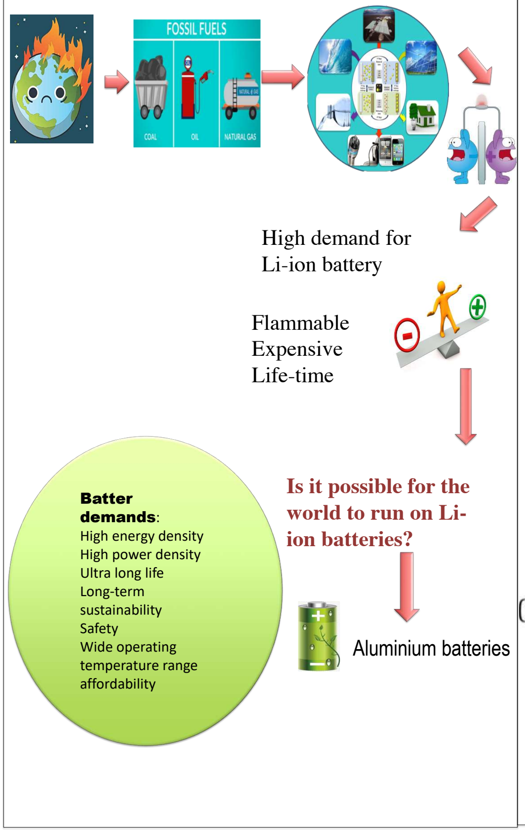
RESEARCH AREA : Non-aqueous rechargeable battery for energy storage devices

ABSTRACT:

With the expanded interest in energy assets, developments in examination and progression have been committed to create progressed energy capacity and conversion systems. Graphene and graphene based materials stand out enough to be noticed inferable for their remarkable properties at high mechanical adaptability, enormous surface region, compound steadiness, unrivalled electric and warm conductivities that render them extraordinary decisions as elective cathode materials. Although Lithium ion batteries (LIBs) have wide applications in the various fields , the deficiency of Lithium assets and risk of combustible electrolytes have restricted their further turn of events. Therefore, an alternative to LIBs in high demand for future energy storage is Aluminium ion batteries(AIBs) . Hence, the poster reviews the latest advancement in graphene based materials for non aqueous Aluminium ion battery.

INTRODUCTION:



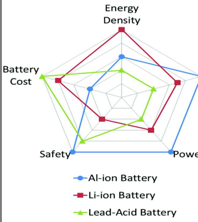
High demand for
Li-ion battery

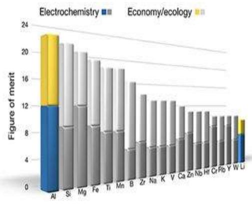
Flammable
Expensive
Life-time

Is it possible for the world to run on Li-ion batteries?

Aluminium batteries

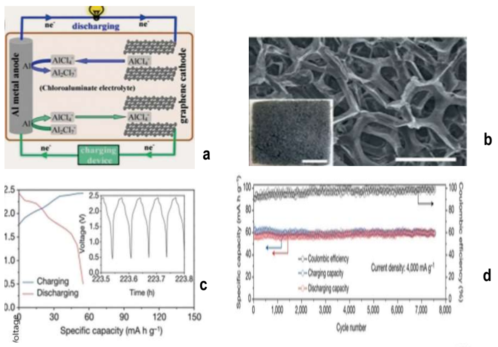
Batter demands:
High energy density
High power density
Ultra long life
Long-term sustainability
Safety
Wide operating temperature range
affordability

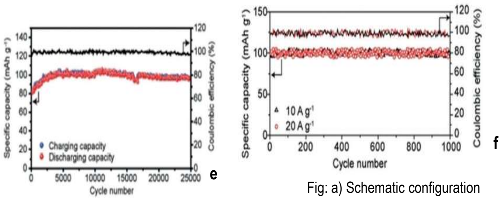




Graphene
- Exotic properties
- Potential applications
- Discharge potential (>1.8V)
- High efficiency
- High discharge capacities at high current rates.
- Outstanding stability
- High thermal tolerance

ELECTROCHEMICAL INVESTIGATION:





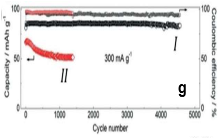


Fig: a) Schematic configuration of Al-graphene cell b)SEM image , cyclic performance c) Al-graphene e)defect free graphene g)different size graphene f) e)defect free graphene at powder form d)GCD profile

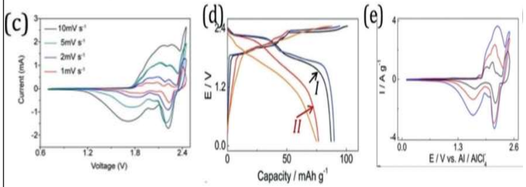
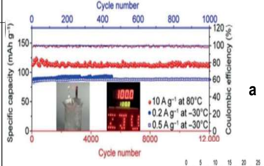


Fig: CV of c) defect free graphene,e) different sized graphene d) GCD of different sized graphene

RESULTS AND DISCUSSION:

Al-graphene battery performance:
- High power density (175 kWkg^{-1})
- Moderate Energy density (66Wkg^{-1})
- Extraordinary fast recharging(1.1-60sec)
- Specific capacity(60-110 mAhg^{-1})
- Ultra long life with negligible loss in specific density at immensely high current rate of 100 Ag^{-1})
- High thermal and mechanical tolerance minimising the risk of safety hazards.



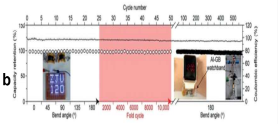


Fig: CV at different a) temperature b) bending conditions.

COMPARISON:

Cathode material	Discharge voltage (V)	Storage capacity[a] (mAh g^{-1})	Current rate (mA g^{-1})	Cycle no.
Graphene foam	ca. 1.8	60	4000	7500
Graphene film	ca. 2	110	10000	250000
Graphene powder	ca. 2	100	5000	5000
V_2O_5	0.5	273	125	20
VO_2	0.5	116	50	100
Ni_3S_2	1	60	100	100
TiS_2	ca. 0.5	30	5	50
Mo_6S_8	0.55	70	12	50
CuS	ca. 0.8	90	20	100
Li_3VO_4	0.5	ca. 50	20	100
V_2CT_x	ca. 1	ca. 100	100	100

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P29

A Theoretical Study of Solid Electrolyte Interphase (SEI) Film Formation in Lithium-Ion Batteries

A Theoretical Study of Solid Electrolyte Interphase (SEI) Film Formation in Lithium-Ion Batteries Nehzat Safaei 1 , F elix Hanke2 April 20, 2022 [1] Dassault Syst`emes, Cologne, A-3, Germany [2] Dassault Syst`emes, Cambridge, CB4 0WN, United Kingdom Electrolyte reduction during the initial charging cycle of batteries, which results in forming of an Electrode-Electrolyte layer, is known to have a considerable impact on the performance of Lithium-Ion Batteries (LIBs) with liquid electrolytes [1-3]. Therefore, understanding of Solid Electrolyte Interphase (SEI) formation mechanism with high resolution is crucial for the improvement of performance of Lithium-Ion batteries. Although SEI formation is investigated extensively with a wide range of experimental technics, the kinetics and the mechanisms of this process are poorly understood, especially at atomistic resolution where there is a technical limitation on the available experimental tools. Therefore, theoretical calculations complementary to experiments, can provide new insights into the electrolyte decomposition which in turn will lead to improvement of battery design. In this research, to investigate the mechanism of SEI film formation in LIBs, we performed atomistic simulations on the carbon anode + ethylene carbonate (solvent) and LiPF6 (salt) as electrolyte, by implementing hybrid MC/MD method [3]. In this method, to overcome the timescale problem of Reactive Molecular Dynamics simulation, we combine Metropolis Monte Carlo and Molecular Dynamics to kinetically sample the systems' events. In our work, first using Quantum Mechanical calculation, we characterize the reaction path of potential pathways which the system can undergo during the anode electrolyte interaction. Then, employing MC/MD simulation we calculate the rate of products' generation during SEI film formation processes and then the mass density distributions in the resulting SEI film is obtained. Based on these results, we provide new insights into the rate of salt and solvent decomposition in (ethylene carbonate + LiPF6) electrolytes. Our calculation suggest a two-layered structure on anode's surface, with an inorganic layer close to the anode and an outer organic layer. References [1] Agubra, V. A.; Fergus, J. W. The formation and stability of the 704 solid electrolyte interface on the graphite anode. J. Power Sources 705 2014, 268, 153162 [2] Bryngelsson, H.; Stjerndahl, M.; Gustafsson, T.; Edstr¨om, K. 707 How dynamic is the SEI? J. Power Sources 2007, 174, 970975. 708 [3] Edge, J. S.; et al. Lithium ion battery degradation: what you need 709 to know. Phys. Chem. Chem. Phys. 2021, 23, 82008221 [4] Abbott, J. W.; Hanke, F. J Chem Theor Comput. 2022 18, 925-93

P30

A perspective on the use of physics-inspired machine learned molecular fields on battery physics

Batteries are the main player in pushing forward the automotive industry and playing a fundamental role in the transition to clean energies. Even though a great amount of work has been done, a particularly pressing issue remains, the understanding of the dynamical properties of battery elements. For example, performing predictive atomistic simulations to generate temperature- and stress-dependent diffusion of ions in materials considering large supercells (several thousands of atoms) using ab-initio-comparable quality energies and forces. The development of machine learned (ML) molecular force fields (FF) during the last ten years has contributed to nano-scale simulations of conventional materials. Nevertheless, the description of the highly complex and fluxional environments in batteries is beyond the reach of conventional ML models. Here, I'll present a perspective on the potential use of new generation ML-FFs and how physics-biased models should be the developing direction to accurately describe, for example, materials densely packed with ion or ions in electrolytes.

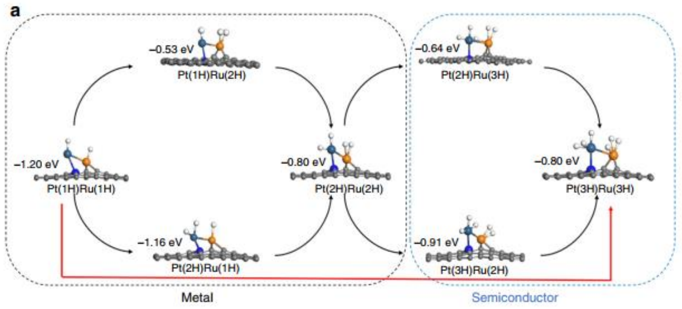
P31

Investigation of orbital regulation mechanism in Single Atom Catalysis

Author: **Rutong Si**

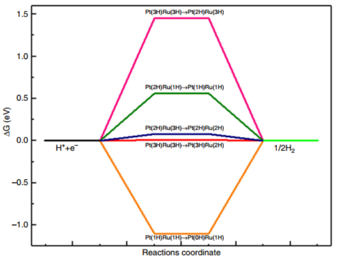
Introductions: Single atom catalysts (SACs), a new frontier in catalysis with the highest atom utilization and abundant active sites, have shown particularly high catalytic activities compared to regular metal nanoparticles (NPs). By decreasing catalyst size to the single atom level, the atom utilization efficiency would be maximized. Simultaneously, the electronic structure of catalysts is tuned by their coordination environment, quantum size effects and the interaction with the support. Thus, SACs usually exhibit distinct catalytic properties as compared to metal NPs. The orbital regulation mechanism play an important role in both SA-support and SA-adsorbates interactions. Pt-Ru bimetallic catalysts and different types of Nitrogen-doped supported Pt single atom are intensely studied as the prototypical SA catalyst model. The SA-support and SA-adsorbates interactions are systematically investigated using DFT calculations. After investigations, several main discoveries are listed here: a) The interactions between H and Ru could be modulated by the Pt through the synergetic effects; b) The adsorbate orbital induced effect is the origin of high HER activity of nitrogen doped support Pt SA.

Pt-Ru dual dimers and their active sites for HER

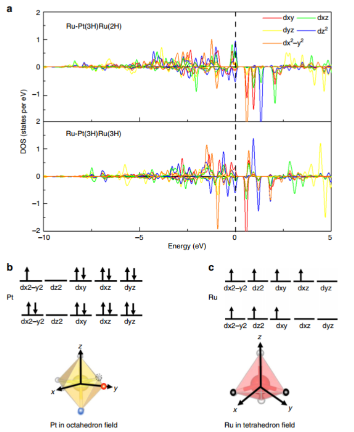


Hydrogen adsorption configurations on Pt-Ru dimer are considered

Different from the NPs, each Pt or Ru atom of dimer could adsorb more than one hydrogen atoms. Thus, we further studied the total hydrogen number of H adsorption on Pt–Ru, which was gradually increased from 2 to 6. Interestingly, after the first step, the hydrogen atoms first adsorb on the Pt side one by one, after three hydrogen atoms adsorb on Pt side and one hydrogen on Ru side, the next one prefers to stay on the Ru atom in sequence. By repeating this process, the maximum number of adsorbed H atoms on either Pt and Ru atoms reach 3. In the following, we referred it as Pt(nH)Ru(mH). before the final step, two possible mediate structures, Pt(3H)Ru(2H) and Pt(2H)Ru(3H), could be formed, and the Pt(3H)Ru(2H) is the energetically more stable. The bond distance between Pt and Ru atoms increases from 2.38 Å (Pt(0H)Ru(0 H)) to 2.75 Å (Pt(2H)Ru(3H)) with the increase of the H adsorption, while it becomes 2.72 Å for the Pt(3H)Ru(2H), which is about 0.1 Å longer than the last step.



the ΔG_H for different coverages of typical configurations

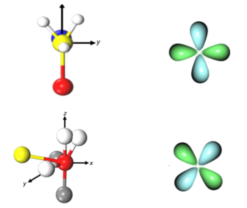


Electronic structures and crystal field of the Ru atom for the last two steps

	dxy(up)	dxy(down)	dyz(up)	dyz(down)	dz2(up)	dz2(down)	dxz(up)	dxz(down)	Dx2-y2(up)	Dx2-y2(down)
32-Ru	**0.92**	0.45	0.75	0.60	**0.92**	0.53	**0.90**	0.49	**0.91**	0.42
23-Ru	**0.86**	0.5	0.71	0.65	**0.91**	0.51	0.72	0.61	**0.86**	0.56
3-Ru	**0.91**	0.39	0.68	0.65	**0.90**	0.57	0.79	0.55	**0.88**	0.58

The occupation number of d-orbital electrons of Pt and Ru

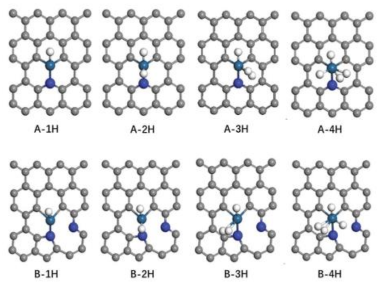
With the further H adsorption on the Ru atom from 2 to 3, the Ru is oxidized from 4^+ to 5^+ and Pt is reduced from 3^+ to 2^+. In this process, the bond distance between the Pt–Ru dimer decreases from 2.72 to 2.63 Å, which results in the electron redistribution between Pt–Ru dimer. The $dx^2–y^2$ of Pt becomes fully-occupied, and the Pt is reduced to 2+. Meanwhile, the bond distance between the Ru with the C atoms of substructure decreases by 0.05 Å. The corresponding bonding between the Ru–C is dyz, thus the antibonding state of dyz is pushed to a rather high energy level (see Fig. 6a). Although $dx^2–y^2$, dz^2 and dxy of Ru remain half-filled, dxz changes from half-filled to fully unoccupied, and the antibonding orbital of dxz is greatly shifted to a rather high energy level. The hydrogen atoms on the Ru atom, exhibiting the smallest ΔGH, just interacts with the dxz orbital for both Pt(3H)Ru(2H) and Pt(3H)Ru(3H). Considering that dxz orbital of Ru becomes unoccupied by the synergetic effect of Pt–Ru dimer during the hydrogen adsorption, the interaction between the hydrogen and the dxz of Ru atom should be rather weak, which should be the main reason why the Pt–Ru dimer exhibits the superior HER as found in our experiment.



Schematic of orbital regulation mechanism of Pt and Ru

Rutong Si, Lei Zhang, Liu L.-M., Xueliang Sun, *Nat. Commun.* 10, 4936 (2019)

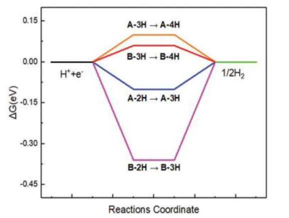
Stability and activity of Pyrrole-like nitrogen doped support Pt SA catalyst



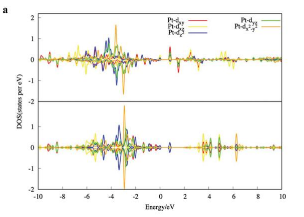
The structure of Pt-HNCNT with the different coverages of hydrogen

After one more hydrogen is adsorbed on the Pt SA, the Pt atom is reduced by the hydrogen from 3+ to 2+, the corresponding oxidation state for Pt are explored based on PDOS and occupation number . The hydrogen heads to the dyz orbital. In this process, the hybridization of N atom is still sp3 and the hybrid orbital tends to be more localized. the s orbital of the absorbed hydrogen atom interacts with the sp3 orbital of the N atom in the pyrrole ring and then forms bonding and antibonding orbitals (Figure a,b). Meanwhile, the dx^2-y^2 and dz^2 remain fully occupied, the dxy and dxz become fully occupied and dyz becomes fully unoccupied (Figure c). The dyz orbital changes from half-occupied to fully unoccupied, interacting with the bonding orbital of H and N atom. Then the antibonding orbital of H and N atom interacts with dx^2-y^2 of Pt atom, which introduces an antibond (Figure b). The hydrogen atom showing the smallest ΔG_H on the Pt atom heads to the dx^2-y^2 orientation. The dyz orbital of Pt SA interacts with the bonding orbital of H and N atom, then the dx^2-y^2 orbital of Pt SA interacts with the antibonding orbital of H and N atom (Figure b). This is stemmed from adsorbate orbital induced effects. Due to the antibonding orbital including dx^2-y^2 orbital of Pt atom and s orbital of H atom, sp3 hybridized orbital is pushed to a rather high energy level by the adsorbate orbital induced effect during the hydrogen adsorption (Figure d). The interaction between s orbital of H atom and dx^2-y^2 orbital of Pt SA should be quite weak. This is the main reason for the superior HER performance exhibited by the Pt-HNCNT in our experiment.

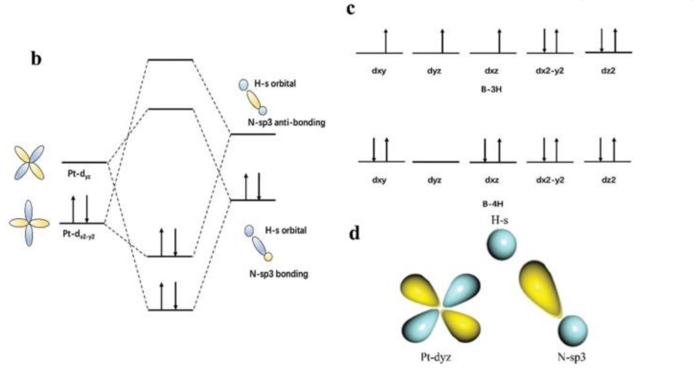
To systematically examine how hydrogen evolves in HER process, the Pt-HNCNT and Pt-NCNT are deeply compared. In the following, we referred the model for Pt-NCNT and Pt-HNCNT in our calculation as A and B Calculations of hydrogen adsorption Gibbs free energy (ΔGH) of Pt-HNCNT were performed to examine the HER activity (Figure b). The ΔG_H of Pt-HNCNT gradually decreases as the number of adsorbed hydrogens increased. Considering the smallest ΔG_H reaches at the highest hydrogen convergence (B-4H), the corresponding oxidation states of Pt atom and orbital interactions between Pt, N, and H atom are studied based on the PDOS. Before the Pt SA reaches the best HER activity on B, one hydrogen atom heads to the dx^2-y^2 and two hydrogens head to dxy and dxz. The hybridization of the N atom in the pyrrole ring is mainly sp3.On this occasion, the dxy, dyz, and dxz are halffilled. The dx^2-y^2 and dz^2 are fully occupied. Here, the hydrogen of the smaller ΔG_H stays primarily in the direction of dxz.



the ΔG_H for different coverages of typical configurations



The PDOS of Pt-HNCNT with the adsorption of three hydrogen



The schematic of the molecular orbital interaction of Pt, N and H atom and the interaction of the dyz orbital of Pt atom, and the hydrogen atom of hydrogen and the sp3 orbital of nitrogen atom

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Simulation software: CP2K Acknowledge: Dr. Lei Zhang, Dr. Fanpeng Kong

P32

Fabrication and functionalization of metal organic frameworks for energy storage applications

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Abstract

Over the time, the depletion of conventional energy resources like fossil fuels and exponentially increasing energy demands promotes the need of renewable energy storage to overcome the global energy crisis. The choice of electrode material depends upon several parameters like high conductivity, sufficient ion storage sites, abundant active catalytic sites, and excellent ion diffusion ability. Among different nanomaterials, metal-organic frameworks (MOFs) have been extensively explored for energy storage applications due to their favorable properties in terms unprecedented chemical properties, structural tunability, and abundant active sites. Present work deals with synthesis of Cu-MOF with controlled size and morphology. Different spectroscopic and microscopic techniques have been employed to characterize the successful synthesis of the Cu-MOF. The electrochemical performance of MOFs and their derivatives majorly depends of facile and controlled synthesis of high-quality MOF. Further, the cytotoxicity of as synthesized MOF is also investigated for real-field applicability

P33

A Force Field for Lithium Diffusion in Crystalline Li7Sn2

P34

Mn-based phosphate framework materials for aqueous Na-ion batteries

Mn-based phosphate framework materials are among the most interesting and sought-after electrode materials for alkali-ion insertion batteries due to their sustainability, high structural stability, and favorable positive electrode potential. However, the search for new Mn-rich materials and their application in batteries remains an open challenge for the research community. We summarize our recent findings and contributions in the search for and applications of novel Mn-based phosphate framework materials suitable for aqueous Na-ion batteries, their structural, morphological, and electrochemical characterization, as well as aqueous stability and degradation issues.

P35

Understanding the effect of doping on the charging performance of the Li-O2 battery: the role of hole polarons and lithium vacancies

In this work, we perform DFT calculations using the hybrid functional HSE to properly describe the insulating nature of lithium peroxide and study its more energetically favourable surfaces [0001], [1 1̄00] and [11 2̄0]. We then analyse how the insulating character and the correct description of the hole polarons at the Li 2 O 2 surfaces affect the electrochemical steps of Li 2 O 2 decomposition in the charging process of the Li-O 2 battery. We then study the effect of doping and propose possible scenarios in which 1the ions as Na + or K + dissolved in the electrolyte can dope and promote Li vacancies generation in the Li2O2 that, in turn, reduce the energy barrier of the limiting steps of the Li2O2 decomposition. The origin of this reduction are the lattice distortions associated with doping that weaken the surface binding.

P36

Structure and dynamics of Ionic liquid electrolytes for lithium ion battery

Developing batteries that have high energy density and safety is of prime importance to meet the emerging challenges in electronics and various energy storage systems. Ionic liquids are gaining widespread recognition as novel green solvents in chemistry. Compared to classical organic solvents, ionic liquids consist of bulky nonsymmetrical organic cations and numerous different inorganic or organic anions. They have wide electrochemical stability window enhanced by a high oxidation potential, and are usually nonflammable and nonvolatile which makes them attractive from the safety perspective. Replacing the flammable carbonate based electrolytes currently being used in lithium ion batteries with nonflammable ionic liquid based electrolytes is considered to be a "hot " research topic. However, their drawbacks are their high viscosity which induces a low wettability of the electrode surface, low ionic conductivity (especially at low temperature), and high cost. In addition, their cations may intercalate interlayers causing mechanical instability to the electrodes, and they might need additives to form stable SEI layer. Knowledge of pure component properties of Ionic liquids is essential but insufficient to determine their applicability for practical use in electrochemical devices. Despite numerous research studies of ionic liquids in lithium ion batteries and a number of experimental and simulation studies of ionic liquid/lithium interactions, the mechanism of ion transport and the nature and size of ion aggregates in ionic liquid electrolytes are still largely unknown. It is unclear yet how the cationic and anionic groups of different Ionic liquids can affect the ionic conductivity as well as the electrochemical stability window of the different solvents.