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8th International Congress on Energy Efficiency and Energy Related Materials (ENEFM 2022)

October 13-19, 2022

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INVITED SPEAKERS

Id-312

Influence of the Synthesis Conditions to Catalytic Activity of the Oxygen Reduction Catalysts

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Abstract: The oxygen reduction reaction (ORR) is a key process for a number of promising electrochemical energy storage devices (EES), such as fuel cells and metal-air batteries. The performance of such devices is limited by the slow kinetics of ORR at the cathode. Low rate of the reaction leads to the necessity of using catalysts. In a common case, the catalysts contain a significant amount of platinum. Platinum catalysts have a high cost and low stability; therefore, the reduction of the platinum content or its complete exclusion from the composition of the cathode catalyst is the main direction in the development of EES technologies using ORR as an electrode reaction.Using alloys of platinum with other metals cannot solve the problem. The catalytic systems based on doped carbon nanomaterials (CNMs) have high activity and stability, then the carbon based catalysts can completely replace platinum catalysts. One of the most prospective ORR electrocatalysts are CNMs doped with nitrogen atoms. These materials are active in both acidic and alkaline electrolytes. It is known that the method of catalyst preparation has a significant effect on its activity in RVC. In this work, we studied the effect of the synthesis conditions of ORR catalysts on their catalytic activity.

Keywords: Oxygen reduction reaction, catalyst, fuel cell, metall-air battery

Acknowledgements: The work was supported by the Russian Science Foundation project #22-13-00035 and using the equipment of the resource centers "Interdisciplinary Resource Center for Nanotechnology" and "Physical Methods of Surface Investigation" of the Science Park of St. Petersburg State University.

INVITED SPEAKERS

Id-359

Biomass Based Renewable Fuel Production Pathways

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Abstract: Depleting petroleum resources, climate change due to excessive fossil fuel consumption, growing global population, increasing standards of living in many developing countries and consumer pleas are the drivers of the increasing demand for products derived from renewable sources and produced with minimal adverse environmental impact. Biomass based biofuel production has the potential to ease the pressure on non-renewable resources for energy production and benefit environment. However, it is critical to ensure that renewable product manufacturing does not compete with food and fiber production for human consumption.This presentation will focus on renewable fuel production from underutilized biological materials and waste streams. Conversion of microalgae grown on wastewater, digested sludge from municipal wastewater treatment facilities and red cedar wood, which is an underutilized lignocellulosic material, to aromatic hydrocarbon enriched bio-oil will be discussed to demonstrate biomass valorization opportunities. An integrated system approach encompassing wastewater treatment during biomass production and utilization of various streams generated within the system will be emphasized. Biodiesel production from microalgae using an eggshell based catalyst and efficiency and quality of biodiesel produced from minimally processed canola oil will be highlighted as potential avenues for promoting decentralized biofuel production at local small-scale facilities.

Keywords: Renewable fuel, biomass, microalgae, digested sludge, lignocellulosic material, biodiesel

INVITED SPEAKERS

Id-368

Optimisation of a Biobutanol Production Process Integrated with a Mixed-Matrix Pervaporation Membrane

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Abstract: Biobutanol typically produced using the ABE (acetone, butanol, ethanol) fermentation process is characterized with low final concentrations and low yield. To remedy this problem, it has been suggested by many researchers to selectively extract butanol from the fermentation broth by integrating a separation process to the fermenter for the in situ recovery such as gas stripping, adsorption, solvent extraction, vacuum distillation, membrane pervaporation. In this investigation, the integration of a mixed-matrix membrane pervaporation separation process with the continuous ABE fermentation system has been simulated and optimized using a multi-objective genetic algorithm. The multi-objective optimisation problem attempts to simultaneously maximize three performance metrics: the overall biobutanol concentration, the butanol productivity, and the sugar conversion while modifying four decision variables, namely the dilution rate, the feed sugar concentration, the cell retention factor and the membrane surface area. The three performance metrics, if non-dominated, define the Pareto domain of the optimisation problem. The optimal solutions of the integrated process were compared to the stand-alone continuous fermentation. By adding an in situ separation system to the continuous ABE fermentation, the optimal butanol productivity and overall butanol concentration increased by approximately 250% compared to those of the non-integrated fermenter. Furthermore, the sugar conversion also increased.

Keywords: ABE fermentation, butanol, optimisation, pervaporation, plate-and-frame membrane module

INVITED SPEAKERS

Id-371

Innovation Drivers in Crystalline Silicon PV Module Technology

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Abstract: Photovoltaic solar energy (PV) is expected to play a key role in the future global sustainable energy system. PV systems consist of many components: photovoltaic modules converting sunlight into DC electricity, inverters changing the electric current from DC to AC, and other accessories to set up a working system (constructions, cabling, monitoring). The key components are PV modules, which are basic devices that are capable of long-term operation in outdoor conditions. PV modules can be implemented from different materials with different production technologies. Innovative driving forces are module cost, module efficiency and module service life. The expansion of technology on a multi-gigawatt production scale also requires minimum material constrains and environment friendly fabrication processes. Changes, which lead to an increase in the efficiency and service life of the modules, can be observed in the field of the starting crystalline material, in the field of the structure and technology of PV cells, in the field of the construction and technology of the modules. New technologies, new materials, and highly productive manufacturing equipment are required to reduce production costs. At present, wafer-based crystalline silicon technologies best meet the criteria due to their high efficiency, low costs, long service life and low material constrains, and in the current production of photovoltaic energy they represent almost 95% of the total module production that this year probably overcame 200 GW_p level in annual production. The influence of individual innovation drivers on the LCOE is discussed. Increasing the efficiency of the modules from 21% to 23% could lead to a reduction of the area-dependent part of the PV system costs by 8.7%. Extending the service life from 25 to 30 years could reduce the LCOE by about 10%. In wafer-based crystalline silicon technologies, a gradual transition from the current PERC technology to higher efficiency cell technologies (HJT, TOPCon) can be expected. Technological innovations make it possible to increase the efficiency of the PV modules closer to the physical limits and to extend the service life of the modules. This transition will depend on the extent to which savings in area-proportional costs outweigh the costs associated with producing modules of higher efficiency, and on overcoming certain material limits that may affect this development.

Keywords: PV module, PV module efficiency, PV module costs, PV module service life, PV module technologies

INVITED SPEAKERS

Id-373

Isothermal Membrane-Based Air Dehumidification: The Material

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Abstract: Air cooling based on the isothermal membrane-based air dehumidification is more energy-efficient and economical than the conventional air-cooling processes. However, there are currently no commercial membrane-based air dehumidification systems due to the limitations of current membranes. Membranes for air dehumidification requires exceptional separation performance, i.e., water permeance $> 10-6\ kmol/m2.s.kPa$ and $H_2O/N_2 > 1000$. In addition, to the excellent separation performance, candidate membranes must possess excellent mechanical reliability and antifouling characteristics. In this presentation, I will introduce membrane-based air-cooling processes, analyze the membrane requirements, review the performance of the current state-of-the-art air dehumidification membranes, and provide a perspective on the research directions. I will also highlight our contributions in developing high-performance air dehumidification membranes based on graphene oxide and mixed matrix membranes. Air cooling based on the isothermal membrane-based air dehumidification is more energy-efficient and economical than the conventional air-cooling processes. However, there are currently no commercial membrane-based air dehumidification systems due to the limitations of current membranes. Membranes for air dehumidification require exceptional separation performance, i.e., water permeance $>10^{-6}$ kmol/s.m^2. kPa and H_2O/N_2 separation factor >1000. In addition, to the excellent separation performance, candidate membranes must possess excellent mechanical reliability and antifouling characteristics. This article discusses the principles and advantages of the membrane-based air-cooling process, analyzes the state-of-the-art air dehumidification membranes' performance, and provides a perspective on the research directions.

Keywords: Air dehumidification, membranes, air cooling

INVITED SPEAKERS

Id-374

Synthesis of Pd Nanodots on 2D $MnFe_2O_4$ Nanosheets for the Cathodic Reduction of CO_2 into HCOOH and Anodic Oxidation of CH_3OH

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Abstract: Direct methanol fuel cell (DMFC) is considered the simplest and most attractive source of energy generation for portable devices and automotive applications that use methanol as a liquid source. In DMFC, liquid fuel, namely methanol (CH_3OH), is electrocatalytically oxidized in the presence of water, resulting in the generation of electricity, hydrogen ions, and CO_2. However, greenhouse gas (GHG) emissions from these devices deactivate the catalyst, resulting in a drastic reduction in DMFC efficiency. In addition, the production of CO_2 during the conversion of methanol is a significant obstacle to the implementation of DMFC on a larger scale. Therefore, the economic and environmentally friendly conversion of greenhouse gasses, especially CO_2, into high-value chemicals is of paramount importance. In this study, spherical-like Pd nanoparticles were successfully grown on two-dimensional $MnFe_2O_4$ nanosheets (2-D Pd/$MnFe_2O_4$ NSs) using microwave irradiation for paired electrochemical reactions. Various characterization techniques were employed to determine the morphological, structural, and chemical properties of the as-prepared bifunctional Pd/$MnFe_2O_4$ electrocatalysts. The 2-D Pd/$MnFe_2O_4$ NSs exhibited higher specific surface area with pore volume, resulting in high CO_2 reduction activity (CO_2RR) for desired formic acid production. By varying the electrolyzer reaction time, cell potential, and electrolyte concentration, we were able to adjust the yield of HCOOH. A Faradic efficiency of (FE) 96.9% was obtained for HCOOH with a maximum yield of 476 mol h^{-1} cm^{-2}. The CO_2RR was also coupled with CH_3OH oxidation (CH_3OH OR) to evaluate the paired electrochemical activity of the bifunctional Pd/MnFe2O4 electrocatalysts. At optimized electrolyzer concentrations, Pd/$MnFe_2O_4$ produced about 625 mol h^{-1} cm^{-2} HCOOH at -1.0 V vs. RHE with FE of 97.5%. A paired electrolyzer increases the HCOOH yield by forming many H+ and e- while CH_3OH OR. The mechanism of the paired electrochemical reaction is described in detail. In this study, it was shown that integrated future bifunctional fuel cells using CH_3OH, in combination with CO_2 reduction strategies, are capable of producing high-value chemicals sustainably without exhaust emissions.

Keywords: Methanol fuel cell, nanodots, anodic oxidation

INVITED SPEAKERS

Id-381

Feasible Routes to Boost Thermoelectricity of *p*- and *n*-type Full-Heusler Compounds

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Abstract: Full-Heusler alloys based on Fe2VAl turn out to bear large potentials for being used in the 100°C temperature range for power generation, cooling, or wireless sensing. Superior power factors (pf) and excellent mechanical properties, the easy synthesis and the non-poisonous and reasonably priced constituting elements, as well as their respective abundance are essential assets in this respect. The present talk aims to focus on various mechanisms which have been employed in order to enhance the thermoelectric performance of such systems. We demonstrate that by modifications of the charge carrier effective mass and the width of the gap in the electronic density of states that pf around 100°C can become 3 times as large, as best performing state-of-the-art materials. A novel mechanism based on charge carrier localization is proposed, boosting the thermoelectric performance and off-stoichiometric sample preparation is employed as well. Our DFT-based calculations allow to perfectly guide experimental studies.

Keywords: Fe2VAl, full-Heusler, thermoelectricity

Acknowledgements: Research supported by the Japanese Science and Technology Agency (JST, Project MIRAI).

INVITED SPEAKERS

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Evaluating Materials for Thermophotovoltaic Emitters

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Abstract: In thermophotovoltaics (TPVs), photovoltaic cells convert heat from a thermal emitter to electricity. One way to obtain high-efficiency devices is to have the emitted spectrum tailored to a specific solar cell. In this work, we propose to use ultra-thin films to tailor the emission of hot bodies. The emitter structures consist of a substrate and a single thin film coating, where we can control the emission spectrum through material choice and film thickness. Considering the optical and thermal properties of 2,809 coating/substrate pairs, we apply this concept to five single-junction TPV systems (GaSb, Ge, InGaAs, and InGaAsSb, and Si). We predict power conversion efficiencies >50%. Also, we suggest new material systems for exploration with potential efficiencies >60%. Our concept is universal and can be expanded to other high-temperature photonic applications for spectral control of thermal emission.

Keywords: Thermophotovoltaics, high temperature photonics, emitters

INVITED SPEAKERS

Id-414

Hybrid Heat Pump Design Strategies to Obtain Net Zero Carbon Buildings

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Abstract: All developed and developing countries seek to take action to avoid the increasingly evident catastrophic impacts of climate change and global warming. Within the University of Derby Zero Carbon Theme these actions are classified as Energy Provision and storage, Manufacturing and Supply Chain, Transport and Smart Cities and Nature based solutions. Geothermal energy has great potential for heating to obtain “Energy efficient buildings “and “Net Zero Energy Building” concepts as defined by European Union. Especially, heat pump applications have shown great improvement in recent years with its commitment to zero carbon buildings. They present a huge potential for hybrid energy efficient applications in the world. This presentation takes in depth look at the current advantages and limitations of Ground Source Heat Pumps (GSHP) and hybrid GSHP design approaches. Although the various design of concepts for the GSHPs available today, it is difficult to find comprehensive information particularly on GSHPs and their hybrid designs. A performance study has been carried out for the ground-source heating system in UK. The actual hybrid ground-source heat pump system design is presented. Moreover, different design strategies for hybrid ground heat pump system are developed and compared from an energy, environmental and economic point of view. This research summarizes the advantages and limitations of GSHP Applications and their hybrid designs, including their future prospects in energy efficient residential, public sector, institutional and agricultural buildings in UK.

Keywords: Energy efficiency, zero carbon, heat pump, hybrid design

INVITED SPEAKERS

Id-415

Conditions for Competitive, Sustainable and Democratic Electricity Systems

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Abstract: Currently, the electricity system in many countries is undergoing significant changes. More and more customers become interested in contributing to their own electricity supply. This was supported especially by the emergence of decentrally applicable technologies such as PV, small CHP and accompanying use of battery storage. The major objective of this paper is to provide insights on how to bring about a competitive, sustainable and democratic electricity system with even higher shares of VRES. Our method of approach is based on the principle of coverage of residual load (= difference between final electricity demand and generation provided by non-flexible electricity generation) on an hourly base over a calendar year based on assumed variable RES generation and development of the load profile; The major results are: (i) Of core relevance is a pricing system in an energy-only market where the price signals provide information about scarcity or excess capacities at every point-of-time; (ii) to balance variations in residual load is a portfolio of flexibility options is important such as: * Battery, pumped hydro and other storage; * Technical demand-side management; * Demand response due to time-of-use pricing. (iii) However, flexible power plants for capacity system adequacy will play a role in every system with and without regulated capacity payments. The major conclusion of this analysis is, that it will be necessary to accept a paradigm shift in our understanding of the whole electricity system where no longer the generators are the centre but coordinating entities such as balancing groups respectively the supply companies. And finally we state that the evolution of such a creative system of integration of RES in Western Europe may also serve as a role model for electricity supply systems largely based on RES in other countries world-wide.

Keywords: Electricity markets, resource adequacy, flexibility, competition

INVITED SPEAKERS

Id-416

Prospects for Renewable Fuels in Road Transport

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Abstract: Transport is still the end use sector with highest increasing emissions and lowest energy efficiency. Fuels based on renewable energy sources (RES) are considered as important means to cope with environmental problems in transport. However, the major problem is that all options of renewable energy use in Transport have pro's and con's. The core objective of this paper is to investigate the perspectives for fuels from biomass, renewable electricity and green hydrogen from economic and ecological points-of-view in a dynamic framework till 2050 for average European conditions. "Renewable fuels" are various First and Second generation biofuels as well as electricity and hydrogen from RES for battery electric vehicles and fuel cell cars. As a reference fossil fuel for comparison we use gasoline in internal combustion engines. The method of approach is based on life-cycle-analyses, dynamic economic assessments (incl. technological learning) and price as well as policy scenarios e.g. for taxes. The major results are: (i) Regarding economics: under current policy conditions – mainly exemption of excise taxes – the economic prospects of biofuels in Europe are rather promising; the major problems of biofuels 1st generation are lack of available land for growing proper feedstocks and the modest ecological performance. Up to 2030 in Europe neither for BF1 nor for BF2 significantly lower costs than today can be expected. Yet, if prices of fossil fuels are increasing further and given current tax policies will become even more competitive. The major economic problem for mobility with hydrogen and electricity are the still very high costs of the corresponding vehicles. By 2050 these costs could be reduced due to technological learning effects and efficient policy measures (e.g. CO2-based tax). (ii) Regarding CO2 emissions: All analyzed fuels have lower CO2-emissions than gasoline and diesel. It is obvious that all categories of electric vehicles contribute to CO2 emission reduction in the tank-to-wheel (TTW) part of the energy supply chain because for all types of battery electric vehicles) (BEVs) and fuel cell vehicles (FCVs) the TTW-CO2-emissions are zero. The largest reduction in total CO2 emission could be reached with BEV powered by electricity from RES and FCV powered by hydrogen produced from RES. To harvest the full environmental benefits of rechargeable EVs and to contribute effectively to heading toward sustainability in transport, it is most important to ensure that EVs use to large extent electricity from RES. All types of biofuels have lower total CO2 emissions than petrol and diesel yet clearly higher ones than BEVs and FCVs based on renewable electricity. The major conclusion is that all types of "clean fuels" will only play a significant role in most countries world-wide if the proper mix of regulation – e.g. emission-free zones in cities – proper CO2-taxes, intensified research & development and corresponding riding down the Learning Curve (e.g. batteries for BEVs and fuel cells) is implemented timely.

Keywords: Renewable fuels, battery electric vehicles, fuel cell vehicles, biofuels, economics

INVITED SPEAKERS

Id-433

Modeling of Catalytic Pyrolysis of Metallized Food Packaging Plastics over Zeolite Catalyst

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Abstract: Metallized food packaging plastics waste (MFPW) is the most complex waste of food packaging. Recently, the pyrolysis treatment has been used to decompose the plastic part of MFPW into paraffin wax product, while the metal fraction (aluminum) remained mixed with black carbon. In order to upgrade the wax products usually, catalytic pyrolysis is used. Within this frame, this research aims to study the catalytic pyrolysis behaviour of MFPW over ZSM-5 Zeolite catalyst with MFPW to catalyst ratios=10, 30, and 50 wt.%. Also, the composition of the obtained chemical compounds was determined using TG-FTIR and GC–MS system. After that, the catalytic pyrolysis kinetic of ZSM-5/MFPW were modelled using linear isoconversional method, distributed activation energy model (DAEM), and an independent parallel reaction kinetic model (IPR). The FTIR and GC-MS results showed that Benzene, Toluene, Hexane, methane, etc. was the main functional group and compounds and their intensity increase as concentration of ZSM-5 increasing. While the kinetics results showed that the activation energies were in the ranges of 174-289 kJ/mol. At the same time DAEM and IPR models succeeded to plot TGA-DTG curves with lower deviations.

Keywords: Metalized food packaging plastics waste, catalytic pyrolysis, LCA

INVITED SPEAKERS

Id-437

Increasing the Efficiency of Sensitized Solar Cell by Doping Natural Flower Dyes of Mountain

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Abstract: Evaluation and Comparison of The Current-Voltage (I-V) Performance for Both Silicon Solar Cells and Dye Sensitized Solar Cell (DSSC) Covered with Natural Plant Dyes, we found that the flowers at top mountains has more efficiency than garden due it resistivity to UV light and it is very stable with constant conversion of solar light to electricity and these natural flowers are cheaper than artificial dyes as they are organometallic dyes.

Keywords: Solar energy, efficiency, natural flower, dyes

REGULAR SESSIONS

Id-336

Salt as a Stable and Cost-Effective Electrode Material for Sodium-Ion Batteries (NIBs)

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Abstract: Sodium chloride (NaCl), initially an ionic compound with a 1:1 ratio of sodium and chlorine ions, breaks all of the basic rules of chemistry at high pressure and forms metallic compounds of Na_3Cl, Na_2Cl, $NaCl_7$, and Na_3Cl_2, which have highly unusual electronic properties and chemical bonding. However, the electrochemical phase transition of NaCl from the insulating state to a metallic has not been achieved yet. In this work, we achieved the metallization of NaCl by inducing Na-ion vacancies in the crystal structure through an electrochemical activation charge process. These Na-ion vacancies cause a phase transition from B1 (Fm3m) to B2 (Pm3m) type NaCl, which could intercalate Na-ions into the structure during the next discharge process, with a high discharge capacity of 267 mAh/g. These intercalated Na-ions will form a 2D-Na layer between alternating layers of B2-NaCl and further charge/discharge process can successfully de-intercalate/intercalate these sodium ions through 2D-layers of B2-NaCl. Meanwhile, this activation charge process also releases Cl-ions from the NaCl structure, which are oxidized to form Cl-based organic species at the active material interfaces. These Cl-based organic species play a crucial role in protecting the NaCl electrode from undesired side reactions at high voltage, resulting in improved cycle retention. To observe the phase transition and de-intercalation/intercalation process of sodium ions, a detailed study was conducted by various *ex-sit*u and *in-situ* analyses. Electrochemical performance proves that metallized Na_xCl: x>1 electrode could show successful de-intercalation/intercalation of sodium ions with a capacity retention of 57 % after 50 cycles. *In-situ* XRD analysis confirms its B1 to B2-NaCl phase transition and sodium intercalation into the structure to form metallic Na_xCl: x>1 phase. Whereas, XPS and XAS analyses are performed to study the breaking /formation of bonding (i.e. Na-Na and Na-Cl interaction) and charge compensation mechanism during the charge and discharge process. XPS, XAS, and TEM–EDS analysis also provide valuable information regarding interphase formation/dissolution on the electrode surface, during the discharge/charge process. Sodium-ion batteries (NIBs) are more cost-effective than lithium-ion batteries (LIBs). However, lowering the cost of the synthesis process of electrode material and battery fabrication is still the main challenge in its commercialization. Due to the natural abundance of sodium chloride as a sodium reserve, NaCl could meet the demands of cost-effective electrodes for large-scale energy storage systems (ESSs) used for the application of renewable energy sources. This work suggests that NaCl, the most abundant and cheapest material on the earth's crust can be used as a metallized-Na_xCl ($x>1$) intercalation system that provides an unlimited opportunity to design electrodes with better performances beyond that of conventional electrode materials of sodium-ion batteries.

Keywords: Sea salt, NaCl electrode, metallic NaCl, Na-ion batteries, capacity retention, cyclability

REGULAR SESSIONS

Id-337

In Pursuit of Novel Material for Providing Renewable and Sustainable Energy via Green Hydrogen Production

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Abstract: Rapid increase in world´s food and energy demand due to global development and population surge led to increase in fossil fuel consumption. The heavy dependence on fossil fuels has not only caused their rapid depletion but also attributed to detrimental environmental issues and emergence of global warming. Hence to preserve human societies and our planet but yet enable sustaining long-term development, there is an urgency to develop renewable and clean alternatives for production of high-value-added chemicals and strategies for energy storage and energy carrier purposes. Coupling renewable sources of energy (such as wind, hydro and solar power) with electrochemical technologies, if done efficiently, could tackle the non-dispatchable nature of renewables by providing storage in chemical bonds. Electrochemical water splitting to produce hydrogen (and oxygen) has been considered to be a clean, efficient, and sustainable strategy to replace fossil fuels. This made hydrogen evolution reaction (HER) an attractive fundamental and practical approach, as it has a fundamental role to play in the production of H_2 electrochemically in a clean and renewable manner. HER is the cathodic half-reaction of water splitting and akin to other evolution reactions, it needs an overpotential to adsorb protons on a surface of a catalyst for the possibility of protons recombination and H_2 evolution. The smaller that overpotential, the better and more promising the catalyst will be. In order to achieve optimum efficiency for HER, activity, stability, and abundancy of the catalyst material are of important factors to consider. To realize industrial-scale H_2 production, substantial challenges on both the fundamental (i.e., catalyst activity and selectivity) and system levels (i.e., mass transport, conversion rate, and energy efficiency) need to be addressed. Here the focus is on the fundamental side where Pt electrode is the best known cathode material for H_2 evolution but Pt is very scarce and expensive and thus other catalyst material needs to be explored which are cheap and abundant and at the same time offer activities close to what Pt has. To address this challenge, state-of-the-art Density Functional Theory (DFT) calculations have been used on modelling new class of electrode materials for the possibility of hydrogen evolution reaction. The H coverage as a function of the applied potential was calculated, and activation energies of H_2 formation at varying conditions was obtained. Surprisingly, similar activation energy of H_2 evolution as on Pt and small overpotential of near zero V to adsorb proton on the surface for initiation of the reaction was found for the Yttrium based catalyst making it interesting for further experimental investigations. This interesting result with more details will be submitted for publication in the proceeding of the ENEFM 2022.

Keywords: Electrocatalytic hydrogen production, DFT calculations, renewable energy

REGULAR SESSIONS

Id-344

Investigation of Oxygen Reduction and Hydrogen Evolution on Cobalt Nanoparticles-Nitrogen-Doped Carbon

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Abstract: In this study, the fabrication of cobalt nanoparticles (CoNPs) supported nitrogen-doped carbon composites using hydrothermal synthesis and their application for oxygen reduction (ORR) and hydrogen evolution (HER) is presented. Scanning electron microscopy (SEM), transmission electron microscopy (TEM), Raman, X-ray diffraction (XRD), and inductively coupled plasma optical emission spectroscopy (ICP-OES) have been used for the characterization of morphology, structure, and composition of the resulting nanocomposites, whereas, the electrocatalytic activity of the ones for the reduction of oxygen and hydrogen evolution in an alkaline medium has been investigated using the rotating disk electrode (RDE). The data for ORR and HER on the CoNPs supported nitrogen-doped carbon catalysts with different Co loadings and structures are presented.

Keywords: Cobalt, nanoparticles, nitrogen-doped carbon, oxygen reduction, hydrogen evolution

Acknowledgement: This study was financially supported by the Lithuanian-Latvian-Taiwanese Tripartite Cooperation Program under the project "Innovate Catalysis for Sustainable Energy (ICatSE)" (P-LTT-21-4, LV-LT-TW/2021/2, MOST 110-2221-E-006-165-MY3).

REGULAR SESSIONS

Id-345

Investigation of Hydrogen Evolution on Cobalt Nanoparticles Supported Graphitic Carbon Nitride

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Abstract: This study is focused on the fabrication of cobalt nanoparticles supported graphitic carbon nitride (CoNPs-g-C_3N_4) composites using microwave and hydrothermal syntheses and their application for hydrogen evolution (HER). The surface morphology, structure, and composition have been examined using X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), and Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES). The electrocatalytic activity of CoNPs-g-C_3N_4 composites for HER has been investigated in 1 M KOH solution. The data of hydrogen evolution on the CoNPs-g-C_3N_4 catalysts with different Co loadings and structures are presented. Compared to the metal-free g-C_3N_4, the doping of g-C_3N_4 with CoNPs enhances the electrocatalytic activity towards hydrogen evolution.

Keywords: Cobalt, nanoparticles, graphitic carbon nitride, microwave synthesis, hydrothermal synthesis, hydrogen evolution

Acknowledgment: This project has received funding from European Social Fund (project No. 09.3.3-LMT-K-712-23-0188) under a grant agreement with the Research Council of Lithuania (LMTLT).

REGULAR SESSIONS

Id-350

Kinetic Modeling of Primary and Secondary Products of Wood Pyrolysis

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Abstract: Pyrolysis plays an integrated role in the biomass conversion processes. Accurate prediction of the yield of pyrolysis products is an important requirement for the design and operation of pyrolysis reactors. A primitive element for the development of sustainable pyrolysis processes is the study of thermal degradation kinetics of waste materials for optimal energy conversion. The study presented here was conducted to predict and compare the optimal kinetic parameters for pyrolysis of woody biomass under isothermal conditions. In this paper, a new kinetic scheme is proposed to predict the composition of pyrolytic products based on Shafizadeh and Chin's model [1] which has been stated to be the most classical model for wood pyrolysis. Our novel model, however, not only involves thermal decomposition of wood into primary products such as gases, tar, and char, and further decomposition of the primary tar into char and gases, but it also models secondary tar (pyrolysis oil). The extent of primary/secondary reactions is varied according to the main process features (temperature, pyrolysis time). The models were numerically solved by using the ode45 solver in MATLAB based on the Runge-Kutta method. The pyrolysis was simulated over the temperature range of 300–500℃ to assess pyrolysis product yields. The yields of pyrolysis oil varied from 45% to 32%, as the percentage of the initial fuel, in the temperature window of 300 to 500℃. The optimum range of production was obtained from our model to be 350-400℃. This agrees well with experimental results showing the optimum temperature range of 350 to 450℃ for the same purpose. The comparison of our model outputs with other models in the literature was satisfactory. Future work will focus on the validation of the model under non-isothermal conditions.

Keywords: Kinetics, pyrolysis, woody biomass, pyrolysis oil, char, gaseous fuel , mathematical modeling

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REGULAR SESSIONS

Id-366

Ahead Scheduling of Controllable Switches and Energy Storage for Optimal Power Flow Considering Forecast Errors

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Abstract: The increase in renewable generation in distribution networks is changing the paradigm for system operators. This paper proposes a methodology to deal with the power flow critical events in the electric distribution grid due to a high penetration of distributed generation and energy consumption. The formulation provides energy peak shaving of the overall system with the integration of Energy Storage Systems (ESS) and a dynamic reconfiguration of Remote Controllable Switches (RCS) to avoid possible power flow violations while taking into account the operational costs of the assets. A multi-objective optimisation is posed to schedule the day-ahead operation of ESS and RCS with a new robust approach to take into consideration the uncertainty of the distributed generation and the load demand forecasts. The non-convex and non-linear mixed-integer problem is solved with a novel combination of the Particle Swarm Optimisation and Genetic Algorithm meta- heuristic algorithms on a 33-bus system.

Keywords: Optimisation scheduling, energy storage systems, distribution 7 network reconfiguration, robust approach, meta-heuristics, smart grids

REGULAR SESSIONS

Id-367

Metal-Organic Frameworks Based on Nickel as an Active Electrocatalyst for Oxygen Evolution from Water Decomposition

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Abstract: Hydrogen is a highly efficient and near-zero-emission energy carrier that, when consumed in a fuel cell, produces only water, electricity, and heat [1]. That is why hydrogen and fuel cells have the great potential to reduce greenhouse gas emissions when providing the biggest amount of energy (by weight) when compared to all known fuels. Finding an efficient catalyst for oxygen evolution reaction (OER) is crucial for productive electrochemical energy storage and conversion from water splitting, due to the sluggish mechanism and high overpotential required [2]. Herein, we report the fabrication of nickel foam impregnated with nickel (Ni-NiF) via a simple one-step route, as a highly active and stable electrocatalyst for OER. We propose a novel structure with promising performance as a replacement for commercially available electrocatalysts. The structure has been studied in depth by state-of-the-art research techniques such as transmission electron microscopy, scanning electron microscopy, Fourier-transform infrared spectroscopy, thermogravimetric analysis, X-ray diffraction and Raman spectroscopy. It was revealed that functionalization with nickel protects the structure of foam allowing it to perform long stability tests at a high current density with lower energy required. The proposed Ni-MOF exhibits an outstanding low overpotential of 292 mV at $10 m\cdot Acm^{-2}$, which is 1.2-fold smaller than commercially used RuO_2 with an overpotential of 360 mV.

Keywords: Electrolysis, electrocatalysts, oxygen evolution reaction, metal-organic framework

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REGULAR SESSIONS

Id-376

Study on Potential and Feasibility of Alternative Fuels Production from Lemon Myrtle Biomass Waste

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Abstract: Nowadays, the acceleration of waste generation from forestry, agriculture and industry is one of the world's critical challenges that contribute to socio-economic and environmental challenges. Specifically, exponential population growth, economic development, and rapid urbanization are the key contributors to waste accumulation which also caused serious environmental problems involving air and water pollution. By utilizing waste from forestry, agriculture and industry, there would be a significant cost reduction in the raw material costs. About a decade ago, Malaysia Agriculture Research and Development Institute (MARDI) introduced a new industrial crop commonly known as Lemon Myrtle, which originated from Queensland, Australia. The essential oil extracted from this crop possesses many benefits as the citrus content is the highest compared to other citrus-containing crops. As for the economic benefits of Lemon Myrtle, it is concluded by MARDI to be more profitable than palm oil. However, no study has been done on the potential of Lemon Myrtle biomass waste as a renewable energy source of feedstock. Thus, managing this waste and upcycling it into valuable products such as solid (biochar), liquid (bio-fuel) and gas fuel can create a circular economy in the pipeline between the commercial and industrial sectors while contributing to carbon reduction. In this study, the processing of tropical plant waste such as lemon myrtle waste into alternative solid fuels with the presence of a natural catalyst was conducted using a microwave carbonized system. Microwave heating technology uses electricity as a source of energy to provide heat for pyrolysis at low temperatures (300 – 500℃) develop a larger amount of biochar and produce side products such as bio-oil and syngas. The syngas will be produced from the carbonization of this biomass at low temperature and the most interesting part, by adding natural catalyst in carbonization reaction, H2 formation was increased while CO, CO2, CH4 and C2H6 percentages are decreased due to the catalyst effect. The effect of the catalyst used on the biochar properties and combustion characteristics was studied through proximate and ultimate analysis while high heating value (HHV) was analysed by using a bomb calorimeter. The biochar products via carbonization of these biomass materials can be characterized as carbon-rich, high heating value and relatively pollution-free potential solid biofuels. The bio-oil products were also presented as environmentally friendly green biofuel candidates.

Keywords: Lemon myrtle biomass waste, natural catalyst, carbonization, microwave carbonized system, biochar, bio-oil, syngas

REGULAR SESSIONS

Id-383

Innovative Geometries for Heat Exchangers: Three-Periodic Schwartz Surfaces

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Abstract: Adsorption heat transformation makes it possible using of heat from low-grade heat sources (solar, geothermal and waste heat) available to the consumer [1]. It is based on a reversible sorption/desorption of sortive vapours with a porous adsorbent. Contact of the dry adsorbent with vapour results in the adsorbent heating and simultaneous cold production in the evaporator. Produced cold and heat can be used by the consumer. The adsorbent can be regenerated by low-temperature heat producing energy-saving effect. The efficiency of an adsorption heat transformer (AHT) depends on the performance of heat exchanger (Hex) where the adsorbent is loaded. The larger the adsorbent mass loaded and the heat transfer surface the better the Hex is. The aim of this study is to look for the optimal Hex geometries to ensure the greater AHT efficiency that will make it possible to give recommendations for the design of more efficient and compact devices.Typical commercial Hex for AHT consists of primary and secondary heat conducting elements that are flat tubes and fins, respectively. Modeling of the geometry of the secondary elements and calculation of their textural characteristics was carried out using a "Creo Parametric" software [2]. The dimensions of the single Hex block were 20x120x7.5 mm^3 (V_Σ = 18 cm^3). The volume V_{ABS} of ABS plastic required for printing of the block and the heat exchange surface area S were calculated. Traditional geometries for secondary elements were the arrays of rectangular plates, tubular squares and hexagonal honeycombs. Another type of secondary elements was three-periodic minimal Schwartz surfaces forming a connected system of cavities [3]. By analyzing the free volume $V_{free} = V_\Sigma – V_{ABS}$ and surface of the elements, the most promising geometries were identified and made by 3D printing. The obtained blocks were placed between flat metal tubes and tested in a laboratory setup to measuring the heat fluxes and the global heat transfer coefficient UA [W/K]. The results demonstrated that changing the geometry of the secondary heat-removing block from a regular (ordinary slot) to a three-periodic (gyroid) leads to the UA increase by 30-40%. This confirms that the periodic Schwartz surfaces are promising geometries for designing of more efficient and compact AHTs.

Keywords: Adsorption heat transformation, energy saving, heat exchanger optimization

Acknowledgment: The work was supported by the Russian Science Foundation (grant 21-79-10183).

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REGULAR SESSIONS

Id-388

Microbial Fuel Cells (MFCs) Developments toward Converting Existing and Future Buildings to Micro-Power Stations and Micro-Treatment Plants

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Abstract: The idea of integrating MFC technology and buildings is very fascinating as buildings will be able to generate the power they need on site. This integrated approach can be widely implemented in both developing countries as well as developed countries, since bricks are ubiquitous. This is a paradigm shift for conventional building concepts, from energy consumer to energy provider (Jiseon You et al., 2019; Jiseon You et al., 2021). Microbial fuel cells (MFCs) are one of the emerging renewable energy technologies, producing electricity from organic matter including waste, using microorganisms. The dual-utility aspect of the technology, i.e., energy recovery from waste whilst cleaning the waste, makes it stand out among other renewable energy technologies. Energy density of an individual MFC unit is relatively low however, thus it is necessary to scale-up to gain a meaningful power output for practical applications. To scale-up, physical stacking and electrical connections of multiple MFC units have been previous suggested (Ieropoulos et al.,2008; Asensio et al., 2017; Gajda et al., 2020). Recent studies have proven that various porous materials can be used as an MFC separator with comparable performance at a much lower cost compared to ion selective membranes (Zhang et al., 2010; Moon et al., 2015; Kim et al., 2016; Winfield et al., 2016; Walter et al., 2022). In this way, a building brick might be able to serve as an MFC separator as well as a chassis. Our study suggests that the idea of converting existing and future buildings to micro-power stations and micro-treatment plants with the help of integrated MFCs and other renewable technologies is achievable, which will be a step closer to a truly sustainable life.

Keywords: Microbial fuel cells, bioreactor, bioenergy, water treatment

REGULAR SESSIONS

Id-391

Water Adsorption Dynamics on the Metal-Organic Framework: Intensification of Heat Transfer in Sorbent Bed

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Abstract: Adsorption heat transformation (AHT) is currently a dynamically developing field of energy. Due to the ability to efficiently use renewable or waste thermal energy sources, AHT systems are considered as energy saving and environmentally benign alternative to common compression those [1]. It is expected that the widespread use of AHT can lead to a significant reducing fossil fuel consumption and associated greenhouse gas emission. Nevertheless, a broader diffusion of this technology is limited by low specific power achievable in actual practice that are mainly determined by dynamics of the adsorption and desorption stages of the working cycle. One of the main factors that influence the sorption dynamics is heat transfer in the adsorbent - heat exchanger unit (Ad-HEx). An efficient route of intensification of heat transfer is the consolidation of sorbent grains with the heat exchanger surface using a binder. A class of porous compounds known as Metal–Organic Frameworks (MOFs) has attracted much attention in recent years as adsorbents for AHT due to the high porosity, huge surface area and tunable sorption properties. MOF-801 is one of the promising water adsorbents for AHT systems, particularly for cooling cycles. It was shown that under adsorptive refrigeration cycle conditions driven by low temperature heat MOF-801 exchanges the amount of water Δw =0.21 g/g and produces the cooling effect at a low temperature of 5°C with an ambient temperature of T_{ads} = 30°C [2]. This work addresses the comparative study of the water sorption dynamic on consolidated layers of MOF-801 and the effects of the binder chemical nature and adsorbent bed configuration on the sorption kinetics and the heat transfer process in the system. Two configurations of the adsorbent bed were studied: (1) loose grains with the size of 0.8-0.9 mm placed on a metal support that imitates a heat-exchanger surface, and (2) layers consolidated with the metal support using different type of binders of organic (polyvinyl alcohol, polyvinylpyrrolidone), inorganic (bentonite) and hybrid (heat-conductive compound) nature. The dynamics of water adsorption on MOF-801 is explored by a Large Temperature Jump method [3] under operating conditions of isobaric stages of adsorptive cooling cycle. It was shown that an initial part of the kinetic curves of water adsorption and desorption obeys the exponential equation $\Delta w(t)/\Delta w(t\to\infty) = 1 - \exp(-t/\tau)$ at a fixed sorption temperature, where $\Delta w(t\to\infty)$ is the final uptake variation and τ is the characteristic time. Based on the obtained results, the effective heat transfer coefficient α between the metal support and the sorbent bed is calculated. It was found that the consolidation of MOF-801 bed with a heat exchanger makes it possible to accelerate the water vapor sorption by heat transfer

improvement. Appropriate recommendation on optimizing adsorbent bed configuration to enhance the AHT power are made.

Keywords: Metal-organic frameworks, MOF-801, water vapor adsorption, adsorption cooling, heat transfer, binder-based adsorbent coating

Acknowledgment:

The work was supported by the Russian Science Foundation (grant 22-23-00659).

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REGULAR SESSIONS

Id-393

Shellmould, A New Concept Of Blank Mold For Glass Contaıners Manufacturıng

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Abstract: Narrow Neck Press and Blow (NNPB) is a process that produces a lightweight container by pressing the glass in the blank mold, baffle, and neck ring to form a parison. In this process, heterogeneous temperature distribution along the molding surfaces is often observed, leading to defects in glass containers. With the significant increase in glass container production, new efficient cooling strategies for improving heat removal and temperature distribution along the molding surfaces are essential to reduce energy consumption and glass defects. This work presents a computational fluid dynamic (CFD) study based on transient simulation of the molding cycle to evaluate the thermal performance of a novel blank mold (ShellMould) for the glass industry. ShellMould consists of two cast iron parts and a conformal cooling channel. Fins placed strategically inside the conformal channel promote heat transfer between the cooling fluid and the blank. A mold with straight cooling channels currently used by the glass industry was considered a reference case model. The mold thermal performance was assessed based on an Indicator of Temperature Heterogeneity (ITH), the heat removal rate, and the average temperature in the molding surface at the blank, baffle seal, and neck ring. ShellMould can reduce the operating temperature by 100 ºC and improve the heat removal rate by 190 up to 202 [J/s]. Results show the main challenges for improving ShellMould cooling and temperature homogeneity, mainly in the neck ring.

Keywords: Blank mold, Glass Industry, Conformal Cooling, NNPB.

REGULAR SESSIONS

Id-408

An Validated Dual-Porosity Approach To Predict Heat Storage in an Aquifer at a Groundwater Remediation Site

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ABSTRACT: Heat storage technologies are essential for the efficient storage of heat from industrial processes or renewable energy sources. In particular, seasonal energy storage is extremely interesting in this respect, as it creates the possibility of transferring large amounts of energy from the summer to the winter months. Underground storage using aquifers to increase storage capacity is one way of storing large amounts of heat over months. Numerical tools are indispensable for predicting the loading and unloading times and the storage capacities to be able to evaluate suitable storage locations well in advance of a cost-intensive exploration of the subsoil. In this paper, we will present the dual-porosity model for the macroscale description of heat and mass transport in heterogeneous aquifers. We will further show how developed cross-scale models can be applied to conduct hydraulic conductivities for different layers in the underground using the framework Pace3D (microscale) and TinFlow (macroscale). In addition, we will show experimentally achieved heat storage test data at a groundwater site in comparison with the numerical results.

Keywords: Dual-porosity, computational fluid dynamics, porosity, underground energy storage, cross-scale numerics

REGULAR SESSIONS

Id-411

Factors Driving Household Solar PV Choices: Differences between Earlier Adopters, Potential Adopters and Non-Adopters

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Abstract: Generating electricity from solar energy is a way for households to participate in the ongoing transition into decarbonized and more decentralized energy systems. A large empirical literature has examined the drivers and barriers associated with household solar PV adoption. An emerging strand of this literature investigates what distinguishes earlier adopters from later adopters and non-adopters. Yet the understanding of the differences between earlier and later adopters remains limited, as few papers have applied formal statistical models to compare the different customer segments. The present study addresses this gap. We examine how the factors that influence household solar PV choices differ between earlier adopters, potential adopters – households that have considered installing solar PV but have not yet done so – and non-adopters. We analyze these choices using a rich data from a household-level survey fielded in Finland. The findings show that the adoption of solar PV is linked to a multitude of socio-demographic and financial factors and personal motivations. There are clear differences in the motives and perceptions of adopters, potential adopters, and non-adopters. Accounting for such differences between customer segments will help better design and target public policy instruments and marketing campaigns that aim to incentivize and nudge households towards solar PV investments.

Keywords: Consumer attitudes, diffusion, adoption, innovations, solar photovoltaic, micro-generation, renewable energy, choice modelling

REGULAR SESSIONS

Id-431

Assessment on SCADA Project Implementation of Electric Distribution Utility for Reliability and Safety in Electric Service

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Abstract: This study assesses the six (6) phases of the three-year implementation of the Supervisory Control and Data Acquisition (SCADA) project for twenty-seven (27) substations of an electric distribution company in Bataan, Philippines, in its pursuit of reliability and safety of power system for better electric service. The assessment aims to measure the degree of improvement in terms of reliability and safety for the accomplished Phase 1 to Phase 6 of the project implementation. The data on power interruption occurrence before and after the implementation of SCADA are assessed using optimization technique to identify the best reliability performance within the various constraints. Furthermore, the data on the response of protection in the substations are also evaluated to see the improvement in safety assemblies of the acquired SCADA. The electric distribution utility involved in this study may use the results in qualifying the relationship between investment and reliability improvement in compliance to national smart grid policy framework.

Keywords: SCADA, substation, electric distribution, reliability

POSTER SESSIONS

Id-308

Recovery of Pgms from Automobile Catalysts as an Important Aspect to Minimize the Amount of Hazardous Waste from Car Industry

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Abstract: Combustion engines are the main driving force for passenger cars, trucks and buses etc. Running engines burn fuel, and as a side effect, release many toxic compounds to the atmosphere. To combat this problem, technical methods were initially applied; their use regulated by laws and regulations. Later on, as environmental awareness among the people increased; it became obvious, that the applied solutions were not enough. This brought the introduction of the first catalytic converters. Nowadays automobile catalyst manufacturing is the largest sector of demand and consumption of PGMs. Without a proper recycling process for spent catalytic converters, they become hazardous waste. Putting them through recycling processes and recovering valuable raw materials not only reduces the amount of hazardous waste, but also reduces the extraction of raw materials from primary sources. According to the latest researches extracting Platinum Group Metals from catalytic converters is much more profitable because 2-5 g of Platinum Group Metals can be obtained from 1 kg of catalytic converters, while extracting Platinum Group Metals from 1 kg of ore gives only 0.002 g. Currently, the level of technology for the recovery of PGMs from catalysts is highly advanced, yet the search continues for solutions that are more sustainable and less harmful to the environment. At the moment, the PHEIDIAS project is working to bring to market an innovative hydrometallurgical process for the recovery of platinum group metals. The technology allows the recovery of platinum at 98%, palladium at 98% and rhodium at 60%. In addition, the technology currently allows work at 70 degrees Celsius, compared to 1,200 degrees Celsius for competing solutions. In addition, the technology uses solvents in low concentrations, which minimizes the amount of waste generated during the entire process. And the efficiency of the process itself allows for processing of 1400 pieces of catalysts, which is about 1 tone. What is worth adding here is the fact that the project is international and it will allow comparing the content of platinum metals in catalysts depending on their origin from a given country. So this will allow us to work out which country is able to supply the largest quantities of PGMs to the market. The aim of this work is to show how the management of used catalytic converters can reduce the waste generation from end-of-life vehicles. At the same time this will show how important it is in terms of a circular economy and the recovery of valuable raw materials from a group of PGMs.

Keywords: Hazardous Waste, Catalyst Recycling, Pgms Recovery, Raw Materials, Circular Economy.

POSTER SESSIONS

Id-318

Numerical Study of Hydrogen Influence on Burning Velocity of Propane-Air Mixtures

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Abstract: Hydrogen influence on flame propagation in H_2-blended propane/air mixtures was investigated by kinetic modeling, using two mechanisms: Warnatz (under INSFLA package) and Gri Mech 3.0 (under Cosilab package). Stoichiometric propane-hydrogen mixtures with various hydrogen concentrations between 0 and 20 vol.% were examined at various initial pressures between 0.5-2 bar, at ambient temperature. The kinetic modelling provided the laminar burning velocities and the profiles of temperature, heat release rate and chemical species concentrations across the flame front. The core elemental reactions and mass fractions of active radicals, which have significant effect on the laminar burning velocity, were analyzed and confirmed. The increase in H_2 content increases the burning velocity of the mixture. This can be assigned to the high reactivity of the H_2 resulting in a higher heat release rate and higher concentrations of active species as compared to non-blended mixtures. This is accompanied by an increase in equilibrium flame temperature and maximum mass fraction of radicals H, OH and O, which in turn determine the increase in laminar burning velocity.

Keywords: Propane, hydrogen, equivalence ratio, burning velocity

POSTER SESSIONS

Id-325

Production of Syngas by CO_2 Reduction through Reverse Water–Gas Shift (RWGS) Reaction over Catalytically-Active Molybdenum-Based Carbide, Nitride and Composite Nanowires

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Abstract: Utilization of renewable CO_2 as a C1 building block is one of the most practical strategies for converting renewable CO_2 into value-added fuels, chemicals and materials. Among the various processes, a highly promising and optimized reaction path is a direct Fischer-Tropsch type process in one reactor with a reverse water gas shift (RWGS) reaction using carbon dioxide in combination with hydrogen as a feed mixture. The feed for Fischer-Tropsch type process can be produced via the RWGS reaction of CO_2.The primary goal of this research was to quantitatively evaluate the catalytic properties in relative conversions rate of CO_2 during the RWGS reaction in a wide temperature range and make a comparison study between these nanowires for the first time. Transition metal carbides and nitrides with large surface areas are attractive for various catalytic reactions. The synthesis of molybdenum carbide, molybdenum nitride and nanocomposite mixed-phase nanowires with the preserved structural morphology of two different precursor reactant materials by heating in diverse gas mixtures is reported herein.Prepared heterogeneous catalysts were characterized using diffraction, physisorption, chemisorption and microscopic techniques. With XRD and interfacial elemental analysis, performed by a transmission electron microscope, the composition of starting intermediate moieties and products was determined. Ordered grain structure appeared almost independent of applied gaseous compounds and typical domain sizes were comparable. The conversions of CO_2 during the reverse water–gas shift (RWGS) were calculated for all measured samples in a wide operation rnge. Composite Mo_2C/Mo_2N showed the highest conversion higher than the pure Mo_2C with similar site amount and especially larger than Mo_2N, which demonstrated a low activity throughout the process. The stability of Mo_2C/Mo_2N wires was tested at 300 °C and they exhibited an unchanged time-on-stream reactivity over a long period of time (>24 h), withstanding deactivation. In addition, the selectivity towards CO was maintained at around 99 %. The comparison of catalyst characterisation before and after RWGS reaction show that there is no major difference in the physical and chemical characteristics of the materials further validate the use of the present catalysts.

POSTER SESSIONS

Id-342

Synthesis of Nanocarbon-Based Materials for Supercapacitors Application

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Abstract: Nowadays, cheap nanocarbon-based materials have been widely used in the energy storage and conversion field. In this study, we present the synthesis of high-efficiency nitrogen-doped carbon materials using kraft pulping residue, black liquor, and wood charcoal as the carbon source. The synthesized catalyst's morphology, structure, and composition were characterized using TEM, XPS, and Raman Spectroscopy. Cyclic voltammetry (CV) and galvanostatic charge-discharge (GCD) techniques have been used to evaluate the electrochemical performance of nanocarbon-based materials. The synthesized nitrogen-doped carbon materials from black liquor and wood charcoal had high specific surface areas of 2481and 2690 m^2 g^{-1}, respectively, and a large volume of pores with an average size of 2.9−4.6 nm. The nitrogen content was ca. 3−4 at.% in the synthesized nitrogen-doped carbon materials. The specific capacitance of ca. 50−80 F g^{-1} has been achieved in the 1 M Na_2SO_4 aqueous solution at the scan rate of 5 mV s^{-1}. Besides, the specific capacitance retention was 99% after 1000 cycles indicating good electrochemical stability.

Keywords: Black liquor, wood charcoal, nitrogen-doped carbon, supercapacitors

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POSTER SESSIONS

Id-346

Testing and Sorting Retired EV batteries

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Abstract: According to automotive standards, the electric vehicle (EV) battery is considered to have reached its end of life (EoL) when it loses between 20%–30% of its initial capacity. This figure is typically acquired by means of a battery management system (BMS) that monitors the battery pack status using key operational parameters such as voltage, current, and temperature. In many cases the reported capacity is limited by the weakest cell or module within the pack that in turn dominates the performance of the whole battery system and hence the EoL decision either in the primary or secondary application. The principle of the recycling hierarchy dictates that reuse be prioritised over repair and recycling thus, in addition to the BMS data a reliable gateway testing strategy is paramount in the battery recycling industry as it aims to provide a piece of detailed information about the status of each individual module or cell. This informs decisions on whether each battery cell/module can be (i) reused in the EV, (iii) reutilised in less demanding applications or is (iii) not economically or functionally viable and must be recycled. In reality, for high volume industrial applications, a gateway testing procedure dedicated to End-of-Life assessment is still in relatively early development stages and requires more work, especially in terms of testing time, cost, and reliability. Therefore, the battery research team at Newcastle University developed a practical sorting method that entails the use of electrical testing metrologies to evaluate the state of health (SoH) of retired battery modules and identifying the degradation mode using partial discharge profile. The feasibility of the proposed method was demonstrated on both 48 lithium-ion battery modules from retired 24 kWh Nissan Leaf battery pack. The experimental results showed that the developed method is capable to estimate the full capacity with a maximum error of 5%. Furthermore, a considerable reduction in the test time is achieved (less than 10 minutes), with only the terminal voltage and discharge current are used, which is of great practical significance to the battery recycling industry where the cost and time are dominant.

Keywords: Lithium-ion batteries, electrochemical-impedance spectroscopy, state of charge, incremental capacity analysis, discharge capacity, battery modules

POSTER SESSIONS

Id-408

An Validated Dual-Porosity Approach To Predict Heat Storage in an Aquifer at a Groundwater Remediation Site

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Abstract: Heat storage technologies are essential for the efficient storage of heat from industrial processes or renewable energy sources. In particular, seasonal energy storage is extremely interesting in this respect, as it creates the possibility of transferring large amounts of energy from the summer to the winter months. Underground storage using aquifers to increase storage capacity is one way of storing large amounts of heat over months. Numerical tools are indispensable for predicting the loading and unloading times and the storage capacities to be able to evaluate suitable storage locations well in advance of a cost-intensive exploration of the subsoil. In this paper, we will present the dual-porosity model for the macroscale description of heat and mass transport in heterogeneous aquifers. We will further show how developed cross-scale models can be applied to conduct hydraulic conductivities for different layers in the underground using the framework Pace3D (microscale) and TinFlow (macroscale). In addition, we will show experimentally achieved heat storage test data at a groundwater site in comparison with the numerical results.

Keywords: Dual-porosity, computational fluid dynamics, porosity, underground energy storage, cross-scale numerics

POSTER SESSIONS

Id-419

Photo-Crosslinked Lignin/PAN Electrospun Separator for Safe Lithium-Ion Batteries

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Abstract: A novel crosslinked electrospun nanofibrous membrane with maleated lignin (ML) and poly(acrylonitrile) (PAN) is presented as a separator for lithium-ion batteries (LIBs). Alkali lignin was treated with a specific esterification agent (maleic anhydride), resulting in substantial hydroxyl group conversion to enhance the reactivity and mechanical properties of final nanofiber membranes. The maleated lignin (ML) was subsequently mixed with UV-curable formulations (up to 30% wt) containing polyethylene glycol diacrylate (PEGDA), hydrolyzed 3-(Trimethoxysilyl)propyl methacrylate (HMEMO) as crosslinkers, and poly(acrylonitrile) (PAN) as a precursor polymer. UV-electrospinning was used to fabricate PAN/ML/HMEMO/PEGDA (PMHP) crosslinked membranes. PMHP membranes made of electrospun nanofibers feature a three-dimensional (3D) porous structure with interconnected voids between the fibers. The cell with 20 wt% of ML PMHP2 membrane had the maximum ionic conductivity value of $2.79*10^{-3}$ S cm^{-1}, which is significantly higher than that of the same cell with the liquid electrolyte and commercial Celgard 2400 ($6.5*10^{-4}$ S cm^{-1}). The enhanced LIB efficiency with the PMHP2 membrane can be attributed to its high porosity, which allows for better electrolyte uptake and demonstrates higher ionic conductivity. As a result, the cell assembled with $LiFePO_4$ cathode, Li metal anode, and PMHP2 membrane had a high initial discharge specific capacity of 147 mAh g^{-1} at 0.1 C and exhibited outstanding rate performance. Also, it effectively limits the formation of Li dendrites over 1000 cycles. The mechanical strength of PMHP membranes with a thickness of 25 µm was enhanced by the variation of the cross-linkable formulations. PMHP separators have improved chemical and physical properties, including porosity, thermal, mechanical, and electrochemical characteristics, compared with the commercial ones.

Keywords: Lithium-ion battery, separator, nanofiber, energy storage, membrane

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	Id 374 - Synthesis of Pd Nanodots on 2D $MnFe_2O_4$ Nanosheets for the Cathodic Reduction of CO_2 into HCOOH and Anodic Oxidation of CH_3OH
	Id 344 - Investigation of Oxygen Reduction and Hydrogen Evolution on Cobalt Nanoparticles-Nitrogen-doped Carbon
	Id 345 - Investigation of Hydrogen Evolution on Cobalt Nanoparticles Supported Graphitic Carbon Nitride
Renewable	Id 359 - Biomass Based Renewable Fuel Production Pathways
Biofuels and Bioenergy	Id 368 - Optimisation of a Biobutanol Production Process İntegrated with a Mixed-Matrix Pervaporation Membrane
	Id 376 - Study on Potential and Feasibility of Alternative Fuels Production from Lemon Myrtle Biomass Waste
	Id 388 - Microbial Fuel Cells (Mfcs) Developments Toward Converting Existing and Future Buildings to Micro-Power Stations and Micro-Treatment Plants
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