

## Working Group on Energy Arbeitskreis Energie (AKE)

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### Overview of Invited Talks and Sessions

(Lecture halls HS HISKP; Poster Tent)

#### Invited Talks

AKE 1.1	Mon	14:30–15:00	HS HISKP	<b>Bedarf und Rolle von Grundlastkraftwerken in einem treibhausgasarmen Energiesystem</b> — ●PHILIPP STÖCKER, BERIT ERLACH, SVEN WURBS, CYRIL STEPHANOS
AKE 2.1	Tue	11:00–11:30	HS HISKP	<b>Energy Studies and Energy Models: A Study Comparison</b> — ●LARISSA BREUNING, ANĐJELKA KEREKEŠ, ALEXANDER VON MÜLLER, THOMAS HAMACHER

#### Invited Talks of the joint Symposium Quantum Science and more in Ghana and Germany (SYGG)

See SYGG for the full program of the symposium.

SYGG 1.1	Tue	11:00–11:05	WP-HS	<b>Welcome Adress</b> — ●BIRGIT MÜNCH
SYGG 1.2	Tue	11:05–11:20	WP-HS	<b>Quantum Education in Ghana</b> — ●DORCAS ATTUABEA ADDO
SYGG 1.3	Tue	11:20–11:45	WP-HS	<b>Mathematical and Computational Physics Research In Ghana: To Cultivate a Knowledge-Based and Sustainable Development Economy</b> — ●HENRY MARTIN, HENRY ELORM QUARSHIE, MARK PAAL, FRANCIS KOFI AMPONG, ERIC KWABENA KYEH ABAVARE, MATTEO COLANGELI, ALESSANDRA CONTINENZA, JAIME MARIAN
SYGG 1.4	Tue	11:45–12:10	WP-HS	<b>Forecasting the Economic Health of Ghana Using Quantum-Enhanced Long Short-Term Memory Model</b> — ●PETER NIMBE, HENRY MARTIN, DORCAS ATTUABEA ADDO, NICODEMUS SONGOSE AWARAYI
SYGG 1.5	Tue	12:10–12:40	WP-HS	<b>Quantum Technology with Spins</b> — ●JOERG WRACHTRUP
SYGG 1.6	Tue	12:40–13:00	WP-HS	<b>Renewable Energy Technologies for Rural Ghana: The Role of Appropriate Technology for Tailored solutions</b> — ●MICHAEL KWEKU EDEM DONKOR

#### Prize and Invited Talks of the joint Awards Symposium (SYAS)

See SYAS for the full program of the symposium.

SYAS 1.1	Thu	14:30–15:10	HS 1+2	<b>A journey in mathematical quantum physics</b> — ●REINHARD F. WERNER
SYAS 1.2	Thu	15:10–15:50	HS 1+2	<b>Precision Tests of the Standard Model at Low Energies Using Stored Exotic Ions in Penning Traps</b> — ●KLAUS BLAUM
SYAS 1.3	Thu	15:50–16:30	HS 1+2	<b>Controlling light by atoms and atoms by light: from dark-state polaritons to many-body spin physics</b> — ●MICHAEL FLEISCHHAUER
SYAS 1.4	Thu	16:30–16:35	HS 1+2	<b>Quantum history at your fingertips: Launch of the DPG's Quantum History Wall</b> — ●ARNE SCHIRRMACHER

#### Sessions

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AKE 1.1–1.8	Mon	14:30–16:45	HS HISKP	<b>Innovative Contributions for the Energy System Transformation</b>
AKE 2.1–2.6	Tue	11:00–12:45	HS HISKP	<b>Processes and Materials for fossil-free Energy Technologies</b>
AKE 3.1–3.2	Tue	14:00–16:00	Tent	<b>Poster</b>

## AKE 1: Innovative Contributions for the Energy System Transformation

Time: Monday 14:30–16:45

Location: HS HISKP

### Invited Talk

**Bedarf und Rolle von Grundlastkraftwerken in einem treibhausgasarmen Energiesystem** — ●PHILIPP STÖCKER, BERIT ERLACH, SVEN WURBS und CYRIL STEPHANOS — acatech - Deutsche Akademie der Technikwissenschaften, Geschäftsstelle, Karolinenplatz 4, 80333 München, Deutschland

Grundlastkraftwerke haben über Jahrzehnte die Stromerzeugung in Deutschland und Europa mit geprägt. Mit dem zunehmenden Ausbau der erneuerbaren Energien nimmt ihr Anteil jedoch aktuell immer weiter ab.

Die vier möglichen Technologien für treibhausgasarme Grundlastkraftwerke werden kurz bewertet in Hinsicht auf ihren Entwicklungsstand, wesentliche Eigenschaften und möglichen Beitrag zur Energieversorgung. Es wird analysiert, wie erforderlich sie in den verschiedenen Dimensionen des Energiesystems in Zukunft sein werden. Die besondere ökonomische Situation für Grundlastkraftwerke wird beleuchtet. Schließlich zeigt die Auswertung von Modellrechnungen auf, welchen Einfluss ihre Präsenz im Modell auf die Zusammensetzung des restlichen Energiesystems und die Gesamtkosten der Energieversorgung hätte.

AKE 1.2 Mon 15:00 HS HISKP

**Optimized transformation planning for municipal energy systems by coupling Agent-Based Modelling and Linear Programming** — ●HANNES KOCH<sup>1</sup>, STEFAN LECHNER<sup>1</sup>, MICHAEL DÜREN<sup>2</sup>, and PETER WINKER<sup>3</sup> — <sup>1</sup>Institut für Thermodynamik, Energieverfahrenstechnik und Systemanalyse, Technische Hochschule Mittelhessen, Gießen — <sup>2</sup>Zentrum für Internationale Entwicklungs- und Umweltforschung, Gießen — <sup>3</sup>Professur für Statistik und Ökonometrie, Justus-Liebig-Universität, Gießen

The transition to climate-neutral energy supply systems is an established necessity. This study provides a framework for detailed optimization and transformation of multi-sectoral energy systems at regional scales and applies it to the county of Giessen, Germany. The methodology combines an Agent-Based Model (ABM) simulating long-term consumer energy choices with a Linear Programming (LP) model that optimizes the economic and climate-neutral transformation of the energy supply system. The ABM incorporates empirical demand data, while the LP utilizes regional renewable energy potential assessments and a pool of available energy technologies to decarbonize the energy supply system. Our findings indicate that the primary drivers of decarbonization are the reduction of final energy demand through renovation of buildings and efficient last-use technologies such as heat pumps and electric vehicles. Additionally, the results suggest that local renewable electricity generation combined with sector coupling presents a more cost-effective and economically resilient solution compared to large-scale renewable energy carrier imports.

AKE 1.3 Mon 15:15 HS HISKP

**Meeting Future Energy Needs - A regulatory view on a sustainability path** — ●JÖRG COSFELD — University of Applied Sciences Düsseldorf, Düsseldorf, Germany

Sustainability demands the cessation of all greenhouse gas emissions to prevent catastrophic climate tipping points. Humanity cannot afford to gamble against these abrupt and irreversible scenarios, which necessitate urgent global political and economic action. This work summarizes carbon dioxide emissions from the energy sector, examining the role of fossil fuels and future expectations. While addressing the challenges of anthropogenic climate change across political, economic, and scientific domains, it highlights the complexity of finding comprehensive solutions.

Rising global energy demands, particularly in electricity generation (40%) and transportation (30%), require solutions that curb emissions. This study explores regulatory frameworks, focusing on the stagnation of American fuel economy progress. From 1975, American Automotive Manufacturers (AAM) improved engine efficiency, enabling greater travel distances per fuel load. However, between 1985 and 2010, due to the lack of updates to Corporate Average Fuel Economy (CAFE) standards, AAM shifted toward heavier vehicles, halting fuel economy improvements.

This work details regulatory gaps and compares fuel efficiency standards in Europe, North America, and Asia-Pacific. It also provides an

outlook on under-regulated sectors requiring scientific and regulatory attention.

AKE 1.4 Mon 15:30 HS HISKP

**Unterwasser-Pumpspeicherkraftwerke in Tagebaugruben** — ●HORST SCHMIDT-BÖCKING<sup>1</sup>, HENRY RISSE<sup>2</sup>, GERHARD LUTHER<sup>3</sup>, JOACHIM SCHWISTER<sup>4</sup> und MICHAEL HOLLERBACH<sup>5</sup> — <sup>1</sup>Uni-Frankfurt — <sup>2</sup>TH-Aachen — <sup>3</sup>Uni-Saarbrücken — <sup>4</sup>Kerpen — <sup>5</sup>Seligenstadt

Die Energiewende in Deutschland steht vor einer großen Herausforderung: Der geplante Zuwachs von Windenergie und Photovoltaik verstärkt die Schwankungen im Stromnetz. Die Kapazität für die Kurzzeitspeicherung elektrischer Energie muss daher dringend und massiv ausgebaut werden. Zurzeit sind weltweit zirka 90 % aller großen Speicher für elektrische Energie Pumpspeicherkraftwerke. Diese Technologie hat sich seit über hundert Jahren bewährt, ist umweltfreundlich und hat einen hohen Wirkungsgrad von bis zu 80 % bei niedrigen Speicherkosten. In Deutschland allerdings steht dem weiteren Ausbau als Hindernis die begrenzte Verfügbarkeit von Standorten entgegen. Eine Lösung dieses Problems stellen wir in diesem Artikel vor: Die bald stillgelegten Braunkohletagebaue bieten aufgrund ihrer beträchtlichen Tiefe ideale Topographien, um das Speicherproblem in Deutschland weitgehend zu lösen. Der Hambacher Tagebau zum Beispiel ist an der tiefsten Stelle über 450 m tief. Folglich muss ein Pumpspeicherkraftwerk für den Einsatz in solchen Gruben anders konzipiert werden, um die vorhandene Tiefe und Größe des Tagebaus zu nutzen.

AKE 1.5 Mon 15:45 HS HISKP

**Modeling of Solid Oxide Fuel Cell and hydrogen storage using Metal Hydrides** — ●ZAHRA HARATI<sup>1</sup>, JAN LOHBREIER<sup>1</sup>, and GHOLAM REZA NABI BIDHENDI<sup>2</sup> — <sup>1</sup>Faculty of Applied Mathematics, Physics and Humanities, Technische Hochschule Nürnberg Georg Simon Ohm — <sup>2</sup>University of Teheran

Multi-energy systems provide extensive benefits over conventional single-source power generation including enhanced efficiency, reduced greenhouse gas emissions, and extended reliability. In the considered multiple system, the solid oxide fuel cell has been selected that can flexibly utilize different fuels, including hydrocarbon gases, coal, and natural gas. In this study, pure hydrogen is produced by PEM electrolysis and stored in lithium borohydride used as fuel in SOFC. Using MATLAB/Simulink, we model the SOFC as a black box using a zero-dimensional approach. The model comprehensively accounts for all SOFC losses, including partial pressure, activation losses, concentration, ohmic losses, and exergy losses, allowing for a complete characterization of the system.

AKE 1.6 Mon 16:00 HS HISKP

**Optical, structural and electrochemical properties of resynthesized Graphite powder for Anode battery application** — ●SLAHEDDINE JABRI<sup>1</sup>, ANNA ROLLIN<sup>2</sup>, SUKANYA SUKANYA<sup>3</sup>, RENÉ WILHELM<sup>2</sup>, MICHAEL KURRAT<sup>3</sup>, UTA SCHLICKUM<sup>1</sup>, and MARKUS ETZKORN<sup>1</sup> — <sup>1</sup>Technische Universität Braunschweig, Institute of Applied Physics, Meldensohn Straße2, 38106 Braunschweig, Germany — <sup>2</sup>Mendelssohnstraße 2 — <sup>3</sup>Technische Universität Clausthal, Institute of Organic Chemistry, Leibnitzstraße 6, 38678 Clausthal-Zellerfeld, Germany

By focusing on preserving the components of Li-Ion battery material through cheaper and environmental friendly methods, recycling process could introduce scavenged impurities into resynthesized material and modify its structural and morphological properties. In this work, we investigate the optical, structural and electrochemical properties of recycled Graphite compared to the new material. Our findings reveal that a proper recycling process can remove the Solid Electrolyte Interphase (SEI) layer, which is of significant importance in battery performance. The analysis showed that proper cleaning can significantly reduce the amounts of organic and inorganic impurities in the graphite, leading to an improvement in material quality. As a result, the battery performance can even be enhanced by 89% after 200 charge-discharge cycles compared to the commercial base material, demonstrating the potential of recycling methods for improving battery life and efficiency

AKE 1.7 Mon 16:15 HS HISKP

**remarkable impact on the structural, optical properties and solar absorbent of ZnO doped into CrNi black coatings** — HANAA SOLIMAN<sup>1</sup>, ABDELSALAM MAKHLOUF<sup>2</sup>, and •DIAA RAYAN<sup>1,3</sup> — <sup>1</sup>Central Metallurgical Research and Development Institute (CMRDI), P.O. Box: 87 Helwan, 11421, Egypt — <sup>2</sup>Engineering, Metallurgy, Coatings and Corrosion Consultancy (EMC3) LLC, Connecticut, USA — <sup>3</sup>Department of Physics, Deraya University, New Minya, Minya, Egypt

Renewable energy is one of the major global challenges towards a clean environment. In solar collectors, high absorption with low thermal emittance represents the main performance parameter during the characterization of the absorber films. This article provides an in-depth study of the co-deposition of Cr and Ni-doped by ZnO coatings and their influence on surface protection correlating it with the absorption of the produced surfaces. Results showed that Cr+Ni+ZnO composite film on Cu substrate outperformed traditional Cr film in terms of surface smoothness, adhesion, corrosion resistance, bending resistance in addition to high solar absorption. Precisely, ZnO inserted into the Cr7Ni3 phase is the key for dual-performance high absorbent and resistant film of CrNi.

AKE 1.8 Mon 16:30 HS HISKP

## AKE 2: Processes and Materials for fossil-free Energy Technologies

Time: Tuesday 11:00–12:45

Location: HS HISKP

### Invited Talk

AKE 2.1 Tue 11:00 HS HISKP

**Energy Studies and Energy Models: A Study Comparison** — •LARISSA BREUNING<sup>1</sup>, ANĐJELKA KEREKES<sup>1</sup>, ALEXANDER VON MÜLLER<sup>2</sup>, and THOMAS HAMACHER<sup>1</sup> — <sup>1</sup>Technical University of Munich (TUM), Germany; TUM School of Engineering and Design, Department of Energy and Process Engineering — <sup>2</sup>Max Planck Institute for Plasma Physics (IPP), Garching, Germany

Energy system models offer insights into a number of areas, such as energy supply, demand for different energy sources, current and future interactions between the supply and demand, interactions between energy and the environment, relationship between energy and the economy, as well as energy system planning, including technology expansion and operation. These models and the implemented scenarios cannot predict the future, but they can show possible paths to achieving a desired goal, emphasize no-regret measures, and explore certain scope and uncertainties. This presentation summarizes published scenario-studies on achieving the goal of climate neutrality by 2045. The transformation paths outlined in the studies are compared with an as-is state and actual developments. Different assumptions and setups are highlighted.

AKE 2.2 Tue 11:30 HS HISKP

**Brave New Nuclear World?** — •FRIEDERIKE FRIESS — Institute of Safety and Risk Sciences, BOKU University, Peter-Jordan-Straße 76, 1190 Vienna, Austria

There are about 400 light-water reactors in operation around the world. The energy they produce is expensive and there are a number of safety issues. Nevertheless, nuclear power is seen by many as an integral part of the future energy system. For nuclear power to make a significant contribution to reducing greenhouse gas emissions, alternative reactor designs must be used. These include small modular reactors (SMRs) and alternative reactor designs often referred to as Generation IV or advanced reactor designs. These reactors are said to produce cheap, safe and reliable green energy. We take a look at the most prominent of these reactor concepts, including reactor concepts such as the sodium-cooled fast reactor (the Russian BN-800 type) and the high-temperature pebble-bed modular reactor, one of which was commissioned in China in 2023. Based on historical experience and available data on advantages and disadvantages, we discuss why this technology cannot be an integral part of the solution to reach net-zero by 2050.

AKE 2.3 Tue 11:45 HS HISKP

**Some Facts on Small Modular Reactors** — •MATTHIAS ENGLERT and CHRISTOPH PISTNER — Öko-INstitut e.V., Rheinstr. 95, 64295 Darmstadt

Small Modular Reactors (SMR) are frequently discussed in the public as relevant for the next decades to reach climate goals and to transition

**Multiscale simulations for the investigation of degradation resistant PEMFC components** — •FABIAN GUMPERT<sup>1</sup>, DOMINIK EITEL<sup>2,3</sup>, OLAF KOTTAS<sup>2,3</sup>, UTA HELBIG<sup>2,3</sup>, and JAN LOHBREIER<sup>1</sup> — <sup>1</sup>Faculty of Applied Mathematics, Physics and Humanities, Technische Hochschule Nürnberg Georg Simon Ohm — <sup>2</sup>Faculty of Materials Engineering, Technische Hochschule Nürnberg Georg Simon Ohm — <sup>3</sup>Institute for Chemistry, Materials and Product Development (Ohm-CMP), Technische Hochschule Nürnberg Georg Simon Ohm

Hydrogen powered technologies provide a huge potential for the transition towards sustainable energy sources, e.g. for mobile applications. However, degradation effects present a significant challenge that currently constrains the practical applications of hydrogen technologies. Proton Exchange Membrane Fuel Cells (PEMFCs) are important devices for the conversion of chemical to electrical energy. For the PEMFC, the Membrane Electrode Assembly (MEA) is a key component, which is especially vulnerable to degradation mechanisms. In this research, we study novel materials for the MEA which counteract these mechanisms and which enable long lifetimes of the devices. The electrode layer is made of composite material, which consists of different components. A multiscale Finite Element Method (FEM) simulation is developed to investigate the composite material used for the electrode layer and to derive practical guidelines for experiments.

to future energy systems. We present data on the technological readiness of and current status of research and development on those reactor concepts and best estimates on their economic viability and timelines for deployment based on sources from literature and the nuclear industry. The focus is both on light water reactor based SMR designs as well as on alternative reactor concepts such as metal-cooled fast reactors, gas-cooled high-temperature reactors and liquid-fuelled molten-salt reactors. For these SMR concepts, extensive research and development work has been taking place for several decades and in some cases since the middle of the last century. Nevertheless, until today no commercially competitive reactor concept exists in the field of SMR. The most extensive technical experience - besides light water cooled systems - is available for sodium cooled and high temperature reactors. However, proof of reliable operation under economic boundary conditions is still required. We finish this talk by summarizing general advantages and disadvantages of the competing SMR systems regarding criteria such as safety, fuel supply and waste disposal, proliferation.

AKE 2.4 Tue 12:00 HS HISKP

**Safety and Licensing Considerations for Small Modular Reactors** — •MARKUS DRAPALIK, FRIEDERIKE FRIESS, and NIKOLAUS MÜLLNER — Institut für Sicherheits- und Risikowissenschaften, BOKU University, Wien, Österreich

Several nations are turning their attention to Small Modular (light water) Reactors (SMRs). Proponents argue that these compact nuclear power plants are both more cost-effective and safer than traditional reactors. The BWRX-300, a 300 MW light water reactor, is one such design with projects planned in Canada and Poland. This presentation delves into the key safety principles underlying nuclear power, such as redundancy and diversity. We will explore how these principles are applied in the preliminary safety analysis report of the BWRX-300, comparing them to the standards used for current (larger) reactors. We further discuss different approaches to fasten the licensing process and in how far those might affect safety. Quick licensing processes are a necessity if nuclear power in general and SMRs in particular are supposed to help significantly in cutting down GHG emissions.

AKE 2.5 Tue 12:15 HS HISKP

**Design and Optimisation of a Variable Reluctance Energy Harvester for Wheel End Caps** — •NIKLAS PÖPEL<sup>1</sup>, YE XU<sup>2</sup>, SEBASTIAN BADER<sup>2</sup>, and JAN LOHBREIER<sup>1</sup> — <sup>1</sup>Technische Hochschule Nürnberg, Nürnberg, Germany — <sup>2</sup>Midsweden University, Sundsvall, Sweden

As vehicular wheel failures are frequently caused by bearing faults, monitoring these components with sensors is very important for effective maintenance. Since the system is rotating, using cables to power the sensors is difficult to implement, whereas batteries only provide

a limited lifetime. Therefore, using a rotational energy harvester as an energy supply is a promising alternative. Previous designs have been proposed that implement a Variable Reluctance Energy Harvester (VREH) within the wheel bearing hub. However, this limits installation to the production stage and leads to complicated repairs.

The aim of this study is to design a VREH that can be installed inside the wheel end cap of large vehicles, providing easier access and lowering the installation costs. To adhere with the requirements of the end cap, an existing VREH design is scaled to the smaller dimensions and structurally inverted. Additionally, geometric optimisations are performed. The new designs are evaluated using a finite element simulation with COMSOL Multiphysics. The results are compared in terms of power output and torque, which helps in finding an optimal design for the VREH at the required scale.

AKE 2.6 Tue 12:30 HS HISKP

**Untersuchung verschiedener auf KI-basierender Ersatzmodelle für 3D FEM Simulationen von thermoelektrischen Generatoren zur Optimierung der Topologie** — EUGEN VAMBOLT<sup>1</sup>, NIKLAS PÖPEL<sup>1</sup>, LILIAN LOWE<sup>1</sup>, LARS FROMME<sup>2</sup>, ELKE WILCZOK<sup>1</sup> und •JAN LOHREIER<sup>1</sup> — <sup>1</sup>Technische Hochschule Nürnberg Georg

Simon Ohm — <sup>2</sup>Hochschule Bielefeld University of Applied Sciences and Arts (HSBI)

Seit Jahren werden diverse Methoden aus dem Bereich der Künstlichen Intelligenz zur Lösung von verschiedensten Aufgaben eingesetzt. Die Vorzüge solcher Verfahren möchte man auch für numerische, physikalische Simulationen nutzen. Bisher werden physikalische Modelle, die auf partiellen Differentialgleichungen beruhen, mithilfe von numerischen Methoden gelöst. Die Berechnungen können dabei je nach Verfahren und Komplexität des vorliegenden Problems bis zu einigen Wochen dauern. Aus diesem Grund werden KI-basierte Ersatzmodelle (\*surrogates\*) aufgestellt. Nachdem die KI-Modelle Informationen aus zum Beispiel Finite Element Berechnungen extrahiert haben, sind sie in der Lage, die Lösungen, die sonst die FEM-Modelle liefern, mit relativ geringen Abweichungen in Echtzeit (1s) zurückzugeben. Die Abweichungen hängen dabei sehr stark von der Anzahl der zur Verfügung stehenden Simulationsdaten und von der Art der KI-Methode ab. Im Rahmen dieses Projektes sollen Ersatzmodelle untersucht werden. Als Anwendungsfall dient die 3D FEM Simulation eines thermoelektrischen Generators, dessen Effizienz maßgeblich von der Topologie des Kühlkörpers abhängt und in dieser Arbeit optimiert werden soll.

### AKE 3: Poster

Time: Tuesday 14:00–16:00

Location: Tent

AKE 3.1 Tue 14:00 Tent

**The Role of Regulatory Frameworks in Reducing Carbon Emissions: Insights from the Energy and Lighting Sectors** — •JÖRG COSFELD — University of Applied Sciences Düsseldorf, Düsseldorf 40476, Germany

Sustainability requires the cessation of carbon dioxide and other greenhouse gas emissions to prevent irreversible and abrupt climate tipping points. This work provides a concise summary of carbon dioxide emissions from the US energy sector and evaluates its greenhouse gas (GHG) abatement potential by 2030. Feasible solutions in a mid-range scenario suggest a reduction of up to 3.0 gigatons of CO<sub>2</sub>-equivalent emissions at costs below 50 USD per ton. Key opportunities lie in energy efficiency improvements and advanced technologies, particularly in buildings, appliances, and power generation, offering both environmental and economic benefits.

The study emphasizes that regulatory frameworks are often better suited for industry sectors than for individual actions, especially in developing countries, where affordability remains a significant barrier. For instance, 5 USD may buy a single LED light but also 10 incandescent bulbs, highlighting the economic trade-offs for low-income households. Comparing US and European regulations, the study discusses the EU ban on incandescent bulbs and Germany's Building Energy Act (GEG), which faced significant public opposition.

In conclusion, regulatory frameworks can effectively support climate change mitigation but require careful design to ensure both practicality and applicability, particularly in economically diverse regions.

AKE 3.2 Tue 14:00 Tent

**Molybdenum-induced modifications in the quantum capacitance of graphene-based supercapacitor electrodes: A DFT study** — •DAVID ANSI, HENRY MARTIN, LINUS LABIK, and ERIC ABAVARE — Department of Physics, Kwame Nkrumah University of Science and Technology, Kumasi, Ghana

Electrochemical Double-layer Capacitors (EDLCs) offer high power density but low energy density due to limited surface area. Graphene, with its high theoretical surface area and capacitance, is a promising material for enhancing EDLC performance. However, the capacity of graphene is restricted by the limited density of states near the Fermi level, resulting in low quantum capacitance ( $C_Q$ ). Doping is a suitable technique for enhancing graphene's  $C_Q$  toward improved supercapacitor efficiency.

Inspired by the molybdenum cofactor, this study investigates molybdenum-induced modifications to graphene's  $C_Q$ . Electronic structures of 15 electrode models were obtained using DFT calculations with the GGA-PBE functional and ultrasoft pseudopotentials in Quantum Espresso. Structures were optimized using the BFGS algorithm with a 3x3x1 supercell for simulations.

The study demonstrates that modifications involving Mo, N, S, and vacancy defects significantly enhance the  $C_Q$  of graphene-based supercapacitor electrodes. The highest  $C_Q$  values were observed when Mo was introduced, due to contributions from Mo's 4d<sup>2</sup> and 4s states. The presence of Mo may introduce pseudocapacitance. These findings highlight Mo-modified graphene as a promising material for EDLCs.