

1 A. ANNUAL HIGHLIGHTS

CAPEX, The Pioneer Center for Accelerating P2X Materials Discovery, carries out fundamental strategic research to provide transformative and scalable solutions for the green transition *by reinventing the ways we invent sustainable materials for Power2X*. Throughout 2023, CAPEX has achieved significant milestones and made substantial progress towards achieving its long-term goals.

Officially launched on May 1, 2023, CAPEX celebrated its scientific opening at DTU on June 28, 2023. The event was attended by representatives from the Danish National Research Foundation and co-funding organizations, key public and industrial stakeholders, and national and international collaborators.

In 2023, CAPEX achieved an important milestone by launching its official website and producing an introductory video about the Center, marking a significant step forward in the Center's outreach efforts. Join the Executive Committee: Director Professor Tejs Vegge and Vice-Director Professor Frede Blaabjerg, as they guide you through CAPEX's vision and groundbreaking research by watching the video, reading our articles, or listening to our podcasts on the CAPEX website: <http://www.capex-p2x.com>.

In the first 8 months, the Executive Committee and Steering Committee, comprising the leads of our research Themes and X-trails, focused on fostering a shared "Pioneering Mindset" among the partners. In addition to coordinating the scientific activities, efforts included recruitment, infrastructure development, and establishing national and international collaborations for PhD and postdoc fellows.

Our first cohort of "Power2Xperts": ten PhD students, five postdocs, and three tenure track Assistant Professors have been recruited. To cultivate a world-leading and sustainable talent pipeline fostering diversity in general and female STEM talent in particular, CAPEX also joined forces with the Velux Foundations, Novo Nordisk Foundation, and "Is it a Bird" to become a *Living Lab* from Nov. 7, 2023.

CAPEX aims to create a unique collaborative and transdisciplinary work environment based on an open exchange of FAIR research data and ideas by locating and integrating the activities on the 3rd floor in the Climate Challenge Laboratory, building 313 at DTU, a uniquely constructed research building dedicated to mitigating climate change. The CAPEX *Transdisciplinary P2X Discovery Lab* has been designed, and the first infrastructure investments have either been made or are well on track.

2023 CAPEX published our first scientific papers and engaged in many dissemination activities, including facility tours, talks, interviews, podcasts, and media articles, as outlined on the website.

As an example, CAPEX researchers contributed to a large international collaboration on developing the first large language machine learning model (MACE-MP-0) for atomistic materials chemistry. This groundbreaking foundation model enables rapid molecular dynamics simulations across diverse materials and molecules, revolutionizing research in the field (<https://arxiv.org/abs/2401.00096>).

CAPEX scientists also secured additional funding from various sources, including NNF, DFF, and EU Marie Curie, for projects spanning CO₂ electrolysis, enzymatic nitrogen reduction, and much more.

In recognition of their scientific contributions to their respective research fields, Anne S. Meyer also received the Foss Research Excellence Award, Anne S. Meyer and Tejs Vegge were honored as Knights of the Order of Dannebrog, Frede Blaabjerg received the Hitachi Energy "Pioneering Spirit Award 2023", and Maria Escudero-Escribano received the Journal of Materials Chemistry Lectureship Award 2021 and the "Extremeños de Hoy" Award.