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SEMICONDUCTORS FOR SUSTAINABILITY: NEXT-GENERATION ELECTRONIC AND ENERGY DEVICES

DILARA ABDEL AND MICHAEL O'DONOVAN

Weierstrass Institute for Applied Analysis and Stochastics (WIAS)
Anton-Wilhelm-Amo Str. 39
10117 Berlin
Germany
abdel@wias-berlin.de , odonovan@wias-berlin.de

Building a sustainable society requires a transition away from fossil fuels toward green energy solutions. At the European level, targets for this transition were set out in the EU Green Deal [1]. This includes the generation of energy from renewable sources, while also electrifying technology which is currently powered by fossil fuels. In parallel, reducing the energy consumption of rapidly growing information and computing technologies must also be addressed. Achieving these goals at a necessary scale will require the development of new materials and devices that combine high performance, long operational lifetimes, and an efficient use of resources.

A variety of technologies will be needed to reach these objectives, including efficient and stable solar cells, batteries, and advanced electronic components. These are united by common mathematical and numerical challenges. The underlying problems include (1) describing similar physical processes across multiple length and time scales, (2) understanding and predicting degradation, (3) identifying relevant parameters for underlying models, and (4) exploring high-dimensional design spaces under multiple objectives.

Addressing these challenges involves a combination of modeling and computational methods at different scales. These include **first-principle approaches** which are limited to small domain sizes, **continuum-based PDE models** which can be scaled to larger systems but may neglect physical effects, and **data-driven techniques** which require a large amount of experimental or accurate simulation data in order to make predictions about new devices.

The goal of this invited session is to bring together researchers from different electronic and energy-device communities to discuss shared mathematical and computational challenges. In particular, we will explore how multiscale modeling, degradation modeling and data-driven methods can be combined to guide device design toward high performance, long lifetime, and sustainable use of resources.

[1] European Commission. *"Communication on The European Green Deal"*. https://commission.europa.eu/publications/communication-european-green-deal_en 2019. COM(2019) 640 final