INTEGRATED COMPUTATIONAL AND EXPERIMENTAL DESIGN OF NEXT-GENERATION BATTERY MATERIALS

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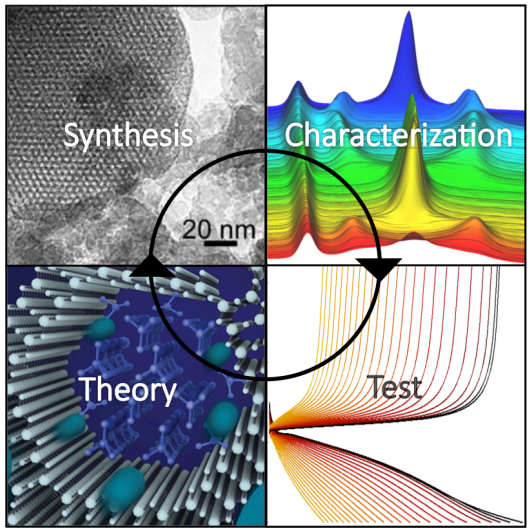
A transition from fossil to renewable energy sources like wind and solar power is of vital importance in the global pursuit of reduced CO_2 emissions. Rechargeable Li-ion batteries offer an efficient solution for short-to-medium term energy storage in portable electronics and advanced Li-ion batteries have now become commercially viable for electric vehicles. The price is, however, generally too high for short-to-medium term grid-scale storage, due to the scarcity and high processing cost of their Co, Mn and Ni content.

With global energy consumption on the scale of terawatts and a growing demand for sustainable transportation, batteries based on scarce materials are not a viable solution. The development of new battery technologies based on more earth-abundant and low-cost materials is therefore a crucial part of a sustainable future energy infrastructure.



Here, we present a number of examples of how a multidisciplinary and highly integrated approach combining advanced computational and experimental approaches can pave the way to the development of next-generation battery technologies, e.g. metal-air, metal-sulfur and all-solid-state batteries. This approach includes new computational methods for accelerated materials design (e.g. combining density functional theory calculations (DFT) with evolutionary algorithms [1]), advanced synthesis methods, simultaneous electrochemical and structural *in situ* characterization (e.g. electrochemical impedance spectroscopy [2] and *in situ* neutron [3] or X-ray scattering [4]) and battery testing, to identify the atomic structure and fundamental processes, which determine the performance of battery materials.

Based on the generated fundamental insight, it is possible to design entirely new battery concepts like nano-confining the solid electrolyte $LiBH_4$ in a nano-porous framework to yield super-ionic Li-ion conductivity and improved cyclic stability [5].

References

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Professor Tejs Vegge from DTU Energy at the Technical University of Denmark (DTU) will present a number of examples of how a multidisciplinary and highly integrated approach combining advanced computational methods like density functional theory (DFT) calculations and experimental *in situ* characterization techniques can pave the way to the development of next-generation battery technologies, e.g. metal-air, metal-sulfur and all-solid-state batteries.

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