AI Accelerated Study of MOF-derived Composites for Supercapacitors

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We utilise predictive modelling and Bayesian optimisation to accelerate the screening process of Metal-Organic Framework (MOF) derived metal oxide-carbon composites to investigate the role of different synthesis parameters in their complex structural and physicochemical properties and electrochemical performance. Batch Bayesian optimisation was implemented for efficiently exploring vast parameter space while maintaining a certain tempo, yet minimising experimental workload and resources needed to achieve such a goal. By choosing exploration, we push our model to go into less performant regions to better understand the design space itself rather to only seek the optimum. Furthermore, we do not only optimise synthesis conditions with fewer trials but also reveal relationships between preparation parameters and electrochemical behaviour by using the trained regression model without the need for extensive experimental data. Hence it is used to evaluate the impact and role of each parameter and linked to corresponding materials properties. Such approach significantly reduces the time and cost associated with materials screening and development, providing a scalable framework to design high-performance energy storage materials and extend insights to broader material systems.

References

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[2] Hussain, Mian Zahid, et al. "Recent advances in metal–organic frameworks derived nanocomposites for photocatalytic applications in energy and environment." Advanced Science 8.14 (2021): 2100625.