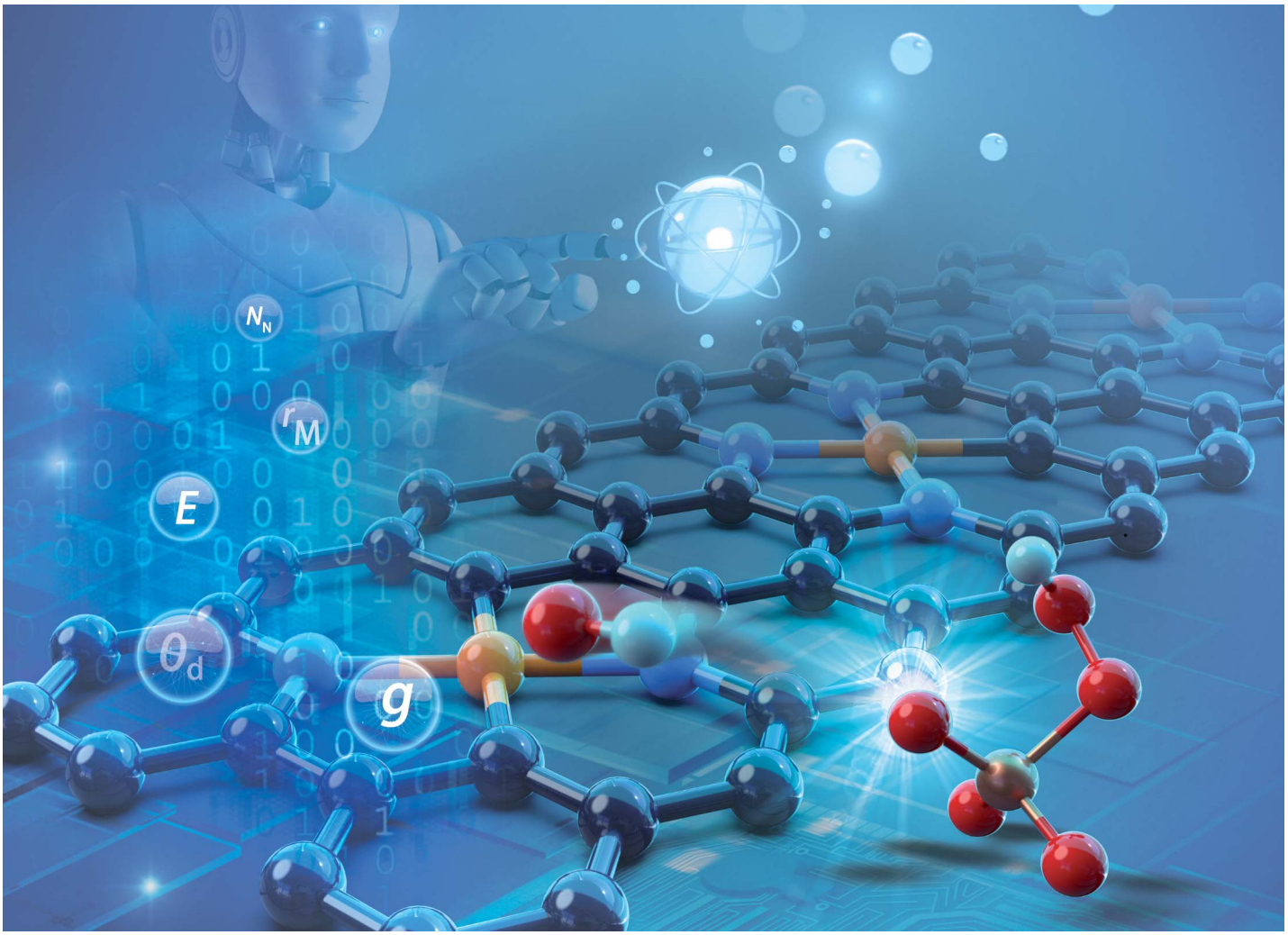
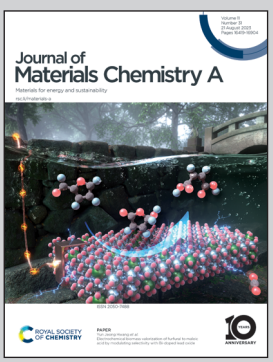


Showcasing research from Professor Zhimin Ao's laboratory, Advanced Interdisciplinary Institute of Environment and Ecology, Beijing Normal University, Zhuhai, China.

Identifying key factors of peroxymonosulfate activation on single-atom M–N–C catalysts: a combined density functional theory and machine learning study

In this work, a series of transition metal-doped single-atom catalysts were used to investigate the intrinsic factors of PMS activation through combining density functional theory and machine learning. A machine learning model was built to reveal the underlying pattern. In descending order of importance, the five electronic and geometric features are group number, d-electron count, electronegativity, radius, and the number of nitrogen atoms. A novel intrinsic descriptor based on these five features was proposed, which can efficiently predict the performance of unknown catalysts.

As featured in:



See Zhimin Ao *et al.*, *J. Mater. Chem. A,* 2023, **11**, 16586.

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