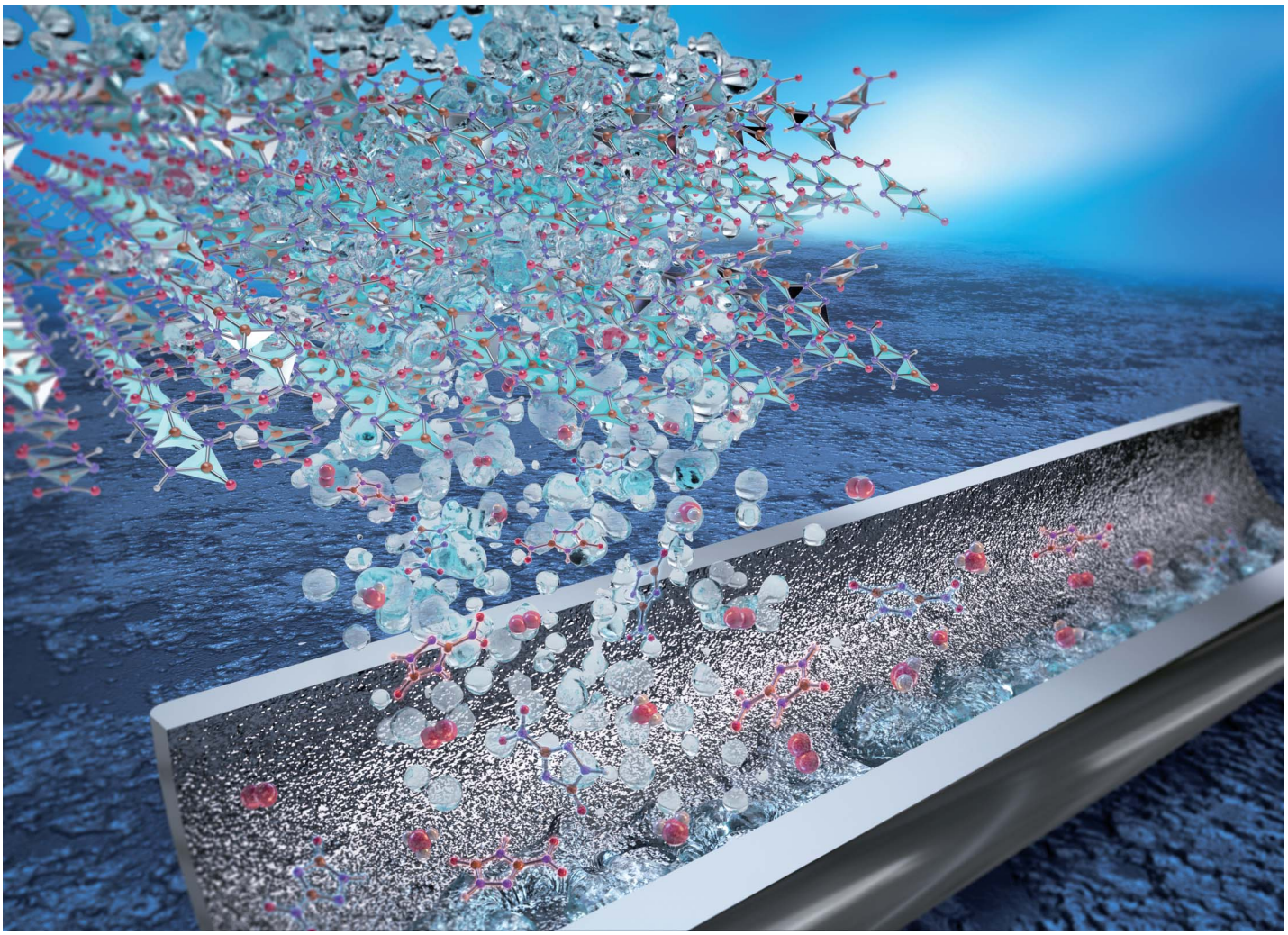
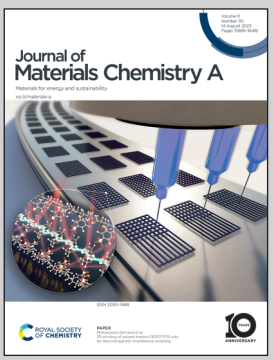


Showcasing research from Professor Qinghai Shu's laboratory, School of Materials Science and Engineering, Beijing Institute of Technology, China.

Unveiling the corrosion mechanism of 3-nitro-1,2,4-triazol-5-one (NTO) toward mild steel from *ab initio* molecular dynamics: how the "nitro-to-amino" reaction matters

The microscopic corrosion mechanism of NTO on the mild steel surface is elucidated through AIMD simulations and enhanced sampling methods. In the presence of Fe(110) catalysis and hydrogen shuttling, both NTO and its anion undergo the "nitro-to-amino" reaction within a 4 ps timeframe, although the reduction barrier for the anion is higher. The surface species (*O and *OH) generated by the "nitro-to-amino" reduction act as corrosion precursors, exacerbating the observed formation of surface iron oxides in the experiments.

As featured in:



See Shuai Zhao, Wei Guo, Qinghai Shu *et al.*, *J. Mater. Chem. A*, 2023, **11**, 16049.

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