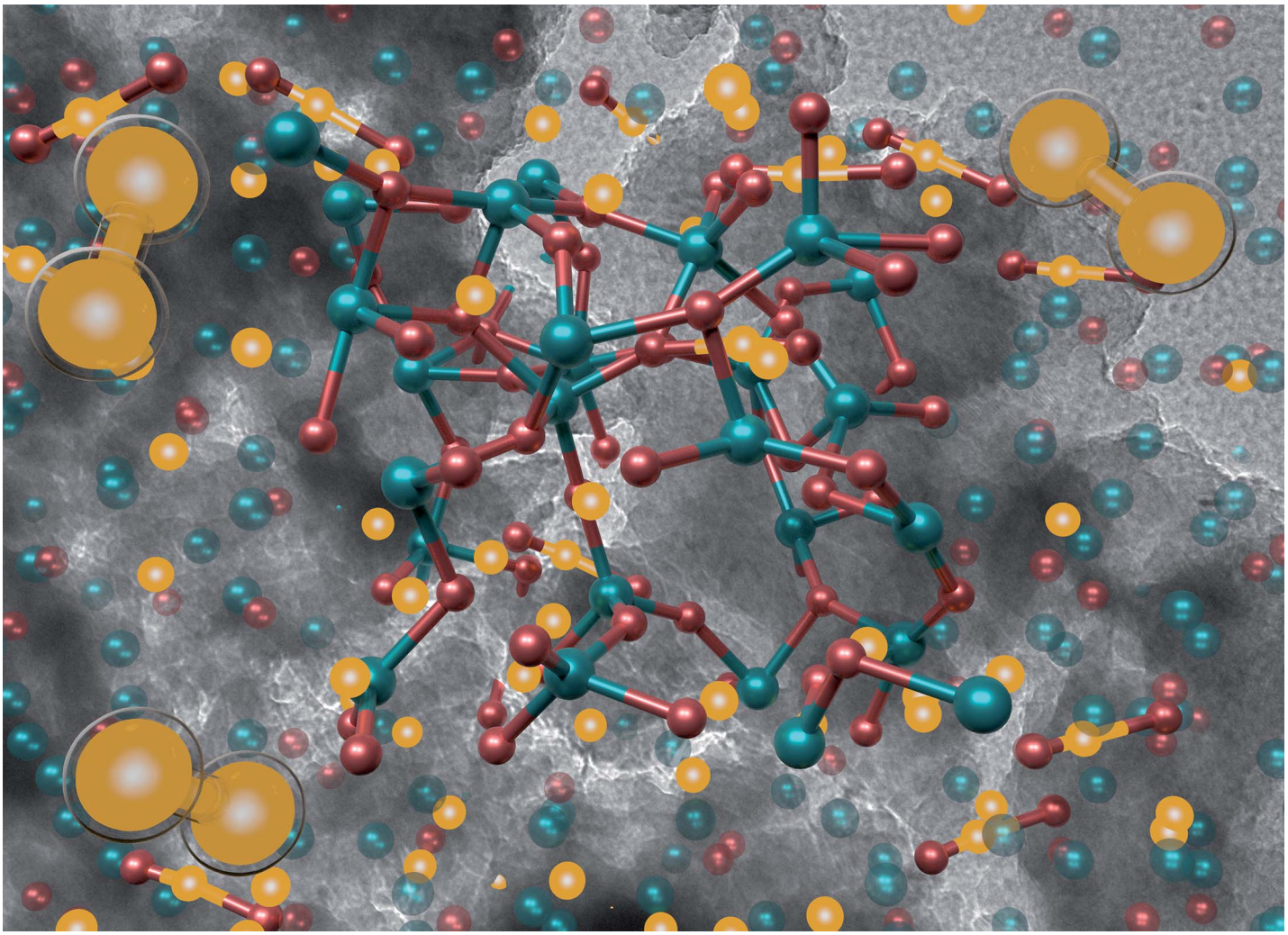
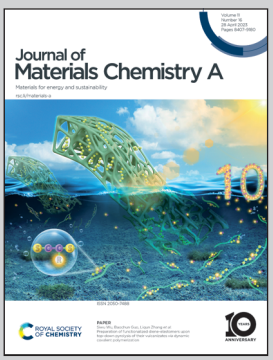


Showcasing research from Lawrence Livermore National Laboratory, Livermore, CA, and Boston University, Boston, MA.

Hydrogen in disordered titania: connecting local chemistry, structure, and stoichiometry through accelerated exploration

Hydrogen incorporation in native surface oxides of metal alloys often controls hydriding, and hence corrosion and hydrogen storage. These oxides tend to be structurally diverse, featuring polymorphic phases, grain boundaries, and amorphous regions. Here, we introduce an integrated computational and experimental workflow that can efficiently and accurately navigate this complexity. We show that hydrogen binding is dictated by local oxygen coordination, which in turn is affected by stoichiometry, and form the basis of transport. This implies that hydrogen incorporation and transport in TiO_x can be tailored through compositional engineering.

As featured in:



See J. Chapman, K. E. Kweon, Y. Zhu, B. C. Wood *et al.*, *J. Mater. Chem. A*, 2023, **11**, 8670.

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