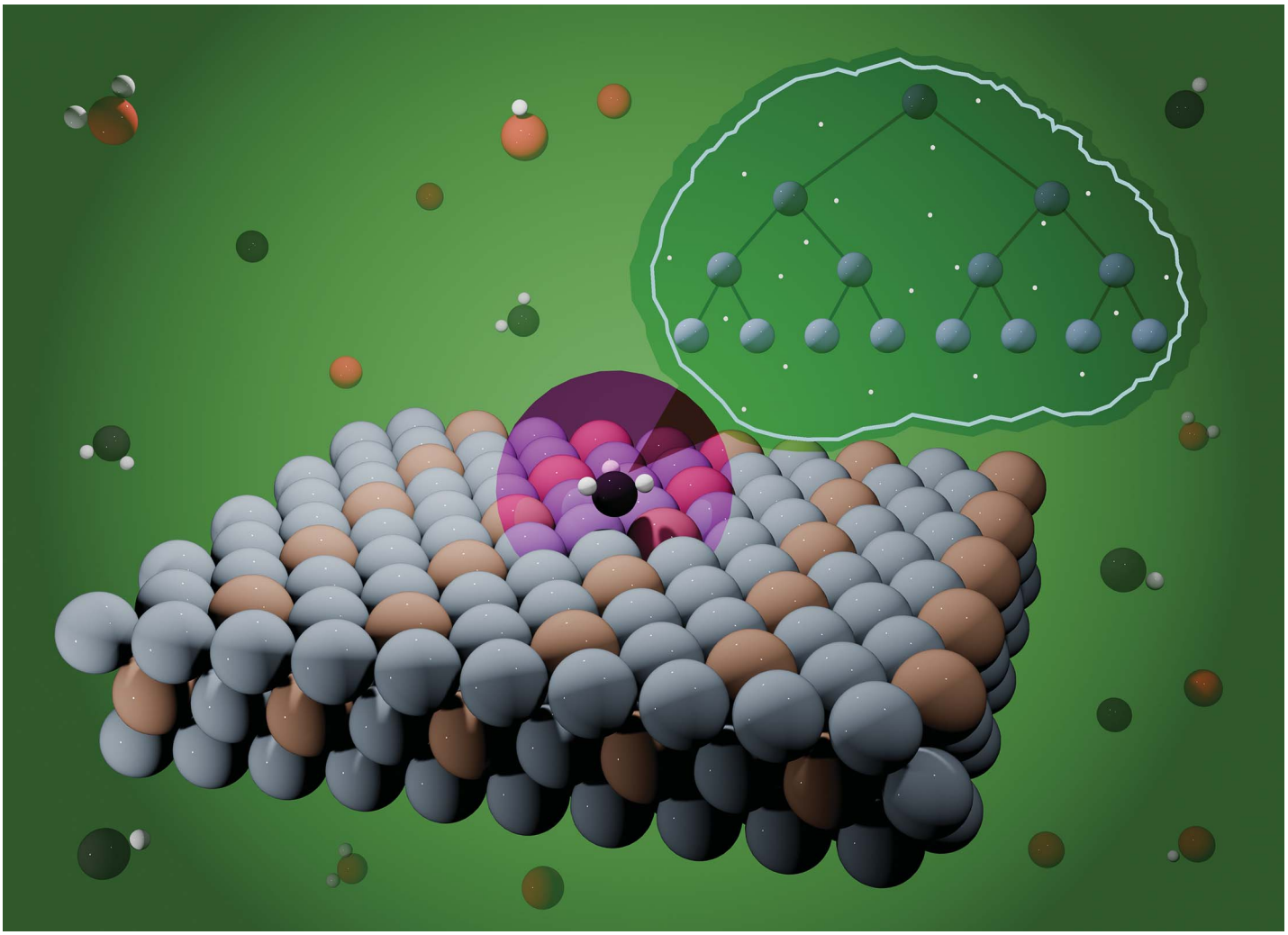
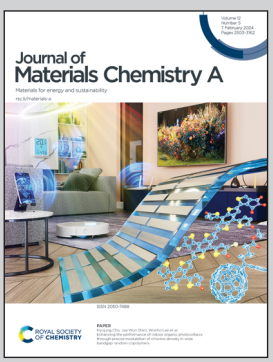


Showcasing the research from Professor A. Comas-Vives from the Institute of Materials Chemistry, TU Wien, Austria, and the Department of Chemistry, Universitat Autònoma de Barcelona, Catalonia, Spain.

Local descriptors-based machine learning model refined by cluster analysis for accurately predicting adsorption energies on bimetallic alloys

A Machine Learning model based on a tree regressor predicts adsorption energies on AB-type bimetallic alloys for species based on C, N, S, O, and atomic H using structural, electronic, and elemental properties. The approach uses local descriptors of the adsorption sites and is refined through cluster analysis. It offers valuable insights into bonding interactions, bringing a valuable tool for screening novel catalytic materials.

As featured in:



See A. Comas-Vives *et al.*, *J. Mater. Chem. A*, 2024, **12**, 2708.

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