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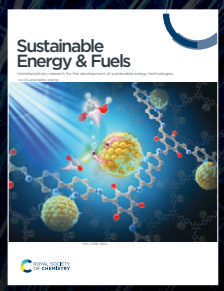

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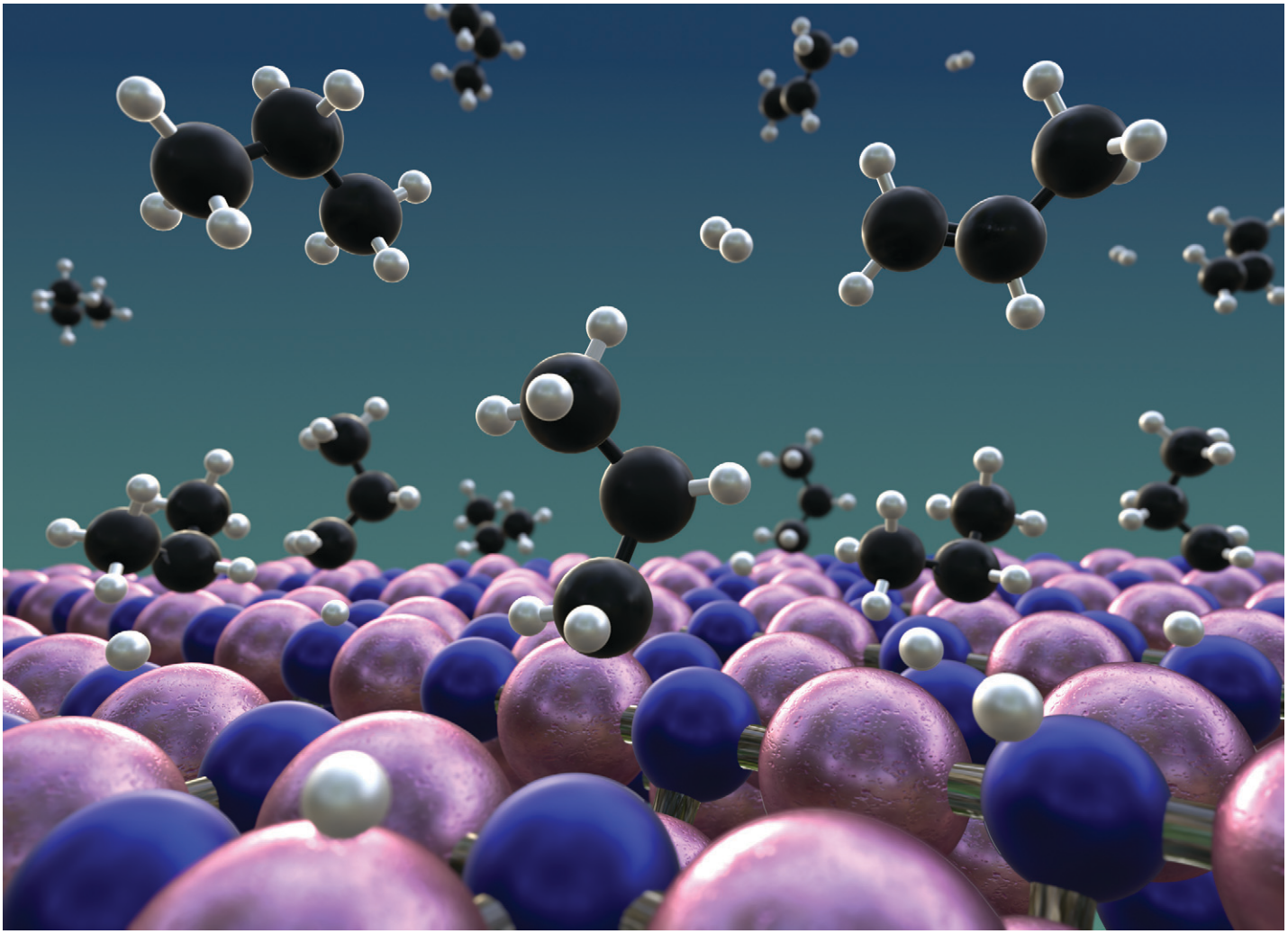

Showcasing research from Professor Giannis Mpourmpakis' laboratory, Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pennsylvania, United States.

Multiscale modeling reveals aluminum nitride as an efficient propane dehydrogenation catalyst

In this collaborative work between University of Pittsburgh and Chalmers University of Technology, computational chemistry calculations were combined with microkinetic modeling and revealed that AlN efficiently converts alkanes to olefins. This study elucidated very complex hydrocarbon dehydrogenation mechanisms and showed that concentration of reaction intermediates on the catalyst surface can play a key role on the preferred mechanism. In addition to providing fundamental understanding of complex reactions, this work aids experiments by identifying catalysts that reduce energy intensity for the conversion of light hydrocarbons from shale gas.

As featured in:

See Giannis Mpourmpakis *et al.*, *Catal. Sci. Technol.*, 2023, **13**, 3527.

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