The Catalytic Dehydrogenation of Hydrocarbons on Metal-Free Graphene

Alastair Brooks[1], Stephen J. Jenkins[1], Marco Sacchi[2]

[1]*Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW, UK*
[2]*Department of Chemistry, University of Surrey, Guildford, GU2 7XH, UK*
m.sacchi@surrey.ac.uk

Carbon-based catalysts have been considered as alternatives to metal-based catalysts and have the potential both to reduce the cost and improve the sustainability of industrial reactions.[1] Novel carbon materials such as graphene offer the opportunity to create catalytic function using carbon itself as the active element, rather than a supporting medium.

In this study, we propose a catalytic mechanism for the dehydrogenation of butane on single-layer, metal-free graphene. Dispersion-corrected Density Functional Theory (DFT) [2] is employed to calculate the transition states and energy minima that describe the reaction-pathways connecting butane to the two possible products, but-1-ene and but-2-ene.[3] The active site for this catalytic reaction is a graphene vacancy (Figure 1), created by removing a carbon atom from a single-layer graphene sheet.

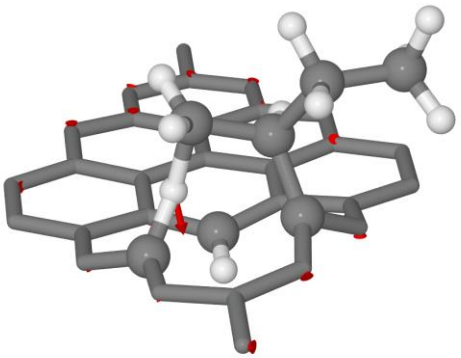

Figure 1. One of the step involved in the catalytic dehydrogenation of butane on metal-free graphene.

The theoretical model of this reaction mechanism not only provides greater insight into catalytic reactions on carbon materials, but it also enables us to assess important features of the reaction, for example the selectivity towards either but-1-ene or but-2-ene.

The results of this theoretical work highlight the possibility of performing a critical and highly activated chemical reaction on the surface of metal-free graphene. This work also opens the route to tuning the dehydrogenation of hydrocarbons on carbon surfaces, whether by modifying the catalyst or changing the reaction conditions.

References:
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