Molecular Diffusion and Reaction on 2D Materials: a First-Principles Perspective

N. F. Xavier, A. J. R. Payne, M. Sacchi

School of Chemistry and Chemical Engineering, Faculty of Engineering and Physical Sciences, University of Surrey, Guildford, GU2 7XH, United Kingdom

m.sacchi@surrey.ac.uk

In the last decade, the surface science community has focused much of its effort on understanding the surface property of 2D materials, in particular graphene. From the technological standpoint, 2D materials have been employed in sensors, optical and electronic devices, membranes, microfluidics, biomedical devices and even in catalysis and electrochemical applications. Although much of the attention around 2D materials is due to their electronic properties, the link between those and the chemical activity of their surfaces and defects is less clear. In our group, we have employed computational methods based on dispersion-corrected density functional theory (DFT) to explore, at the atomic level, the link between the electronic structure of graphene and boron nitride and the behaviour of molecules adsorbed on their surfaces. In collaboration with experimental groups, we investigate the ultrafast dynamics of ammonia and water on graphene and graphite [1-3]. More recently, we have investigated the reactive scattering of NH_3, CH_4 and butane on defective graphene and h-BN and suggested that the vacancies and edges of these 2D materials could be employed as active sites for dehydrogenation reactions [4,5]. Dispersion-corrected DFT seems to work remarkably well in describing the extremely flat potential energy surface of carbon surfaces [7]. We are currently exploring the interaction of small biomolecules with graphene and pursuing novel routes for integrating quantum effects in proton tunnelling over surfaces [8].

[1] Tamtögl, Anton, Nature Communications, **12** (1), 3120 (2021).
[2] Tamtögl, Anton *et al.*, Carbon, **126**, 13 (2017).
[3] Sacchi, Marco and Tamtögl, Anton, Advances in Physics: X, **8** (1), 2134051 (2023).
[4] Payne, Anthony J. R. *et al.*, Physical Chemistry Chemical Physics, **24**, 20426 (2022).
[5] Brooks, Alastair *et al.*, Journal of Colloid and Interface Science, **619**, 377 (2022).
[6] Calvo-Almazán, Irene *et al.*, The Journal of Physical Chemistry Letters, **7** (24), 5285 (2016).
[7] Slocombe, Louie, Sacchi, Marco and Al-Khalili, Jim, Communications Physics, **5** (1), 109 (2022).