

## Physical Organic Chemistry

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Physical organic chemistry is broadly defined and of fundamental importance for the development of interdisciplinary areas that link together chemical synthesis and biological and material sciences with theoretical and physical chemistry. In its classical sense, physical organic chemistry can be defined as the study of mechanism, reactivity, structure, and binding in organic systems, which leads to the quantitative understanding of their properties at the molecular level. Modern physical organic chemistry also encompasses a wider range of contexts and interactions, which extend beyond reaction pathways. Some important current topics include supramolecular interactions and molecular recognition, aggregation and reactivity, computation of reaction pathways, reactions and catalysis in biology, materials where molecular structure controls function, structure activity correlations, mechanisms in synthesis and catalysis, and interactions and reactivity in organised assemblies and interfaces. The program of the Gordon Research Conference on Physical Organic Chemistry (conference title: Understanding Chemical Reactivity – New Concepts and Applications), which was held in June 2013 at the Holderness School, New Hampshire, USA, spanned the wide area of modern physical organic chemistry. This Research Front on physical organic chemistry is dedicated to this highly interdisciplinary field by showcasing research that ranges from mechanistic organic and bio-organic chemistry to materials chemistry.

Fluorescence spectroscopy is a powerful method for monitoring conformational changes in proteins and protein–protein associations. Petersson and co-workers<sup>[1]</sup> describe in their review strategies for labelling proteins with fluorescence probes with a particular focus on evaluating the balance between size and utility of the fluorophores, since large sizes can be disruptive to the protein's fold or function, but on the other hand provides valuable characteristics such as visible wavelength absorption and emission or brightness.

Formation of C–C bonds mediated by transition metals are amongst the most important reactions in organic synthesis. The search for new types of reactions requires a detailed

understanding of the mechanism of these reactions. O'Hair and colleagues have used multi-stage mass spectrometric techniques to obtain mechanistic insight of the cobalt-mediated Glaser-type decarboxylative homocoupling of alkynyl carboxylic acids.<sup>[2]</sup> These studies revealed that dinuclear cobalt clusters are superior to mononuclear complexes at promoting both decarboxylation steps as well as the reductive coupling itself.

Reversible bond formation and dissociation of radical species ( $\pi$ -dimers) in solution phase can be applied to control the mechanical motion of molecules. Nishinaga and co-workers studied the diradical character of benzo- and naphtho-annelated thiophene-pyrrole mixed oligomer dications and their application in  $\pi$ -dimer based supramolecular chemistry.<sup>[3]</sup>

Organic semiconductors have become increasingly important as substitutes for conventional inorganic materials. Jeffries-EL and co-workers have explored the optoelectronic properties of two-dimensional cross-shaped 'cruciform' molecules possessing two extended conjugation axes, which enable independent manipulation of the HOMO and LUMO levels by incorporating electron-donating and -withdrawing substituents at different positions along the two axes.<sup>[4]</sup>

This selection of invited papers in this Research Front is just a snapshot of the variety of research that is currently being performed under the broad category 'physical organic chemistry'. It is this diversity of science and the constant developments that will keep this field exciting in the future.

### References

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Uta Wille graduated with a Ph.D. in science in the field of atmospheric chemistry at the University of Kiel, Germany, in 1993. This was followed by a habilitation in organic chemistry at the same institution, which was completed in 1999. In 1997–98, she undertook a Postdoctoral Fellowship with Professor Bernd Giese at the University of Basel, Switzerland. In 1999, she was appointed as Privatdozent at the University of Kiel and was invited in 2000 as a Visiting Fellow to the School of Chemistry at the University of Melbourne. In January 2003, Uta moved permanently to the University of Melbourne, where she has been Associate Professor and Reader since 2011. Her research program is in the area of physical organic chemistry, where she studies the chemistry of reactive intermediates by merging radicals of atmospheric importance with organic and bio-organic chemistry.