INTERNATIONAL SOLVAY INSTITUTES BRUSSELS

Solvay Colloquium

Prof. Sason Shaik
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Oriented Electric Fields - New Effectors in Chemistry

The talk will discuss the wide-ranging potential of using oriented external-electric-fields (OEEFs) as new effectors of chemical change.[1-5] Generally speaking, an OEEF along the direction of electron reorganization from reactants to products, will catalyze/inhibit at will non-polar reactions, while orientations of the OEEF off the "reaction axis" will control selectivity patterns and chiral discrimination.[1,3] The field's direction will similarly affect bonds, molecular structures and aggregation.[5]

I shall discuss OEEF effects, using a selection from the following topics: (a) Control of bond length and strength, and molecular structures, (b) control, at will, of non-redox chemical reactions by catalyzing or inhibiting them through a flip of the field's direction, (c) control of regioselectivity (e.g., C=C vs C-H activation by oxoiron reagents (e.g., P450 like),[1,5] exo/endo selectivity in Diels-Alder reactions),[1,5] (d) control of spin-state selectivity,[1,5] (e) control of reaction mechanisms,[1,5] (f) the dilemma of electric fields in enzymes,5 and (g) control of chiral discrimination and enantioselectivity.[3] Some future prospects may be discussed as well: (a) the ability of OEEF to act as tweezers that orient the reactants in space and catalyzes their reactions, (b) the role of OEEFs in self-assembly.

As shall be described, there are by now a variety of experimental techniques to implement the OEEF idea,[2,5] including scalable options.[2b] The field is rapidly expanding. As experimental techniques mature further, chemical transformations may become an exercise in zapping oriented molecules with OEEFs.

1 Shaik, S. ; Mandal, D. ; Ramanan, R. Oriented Electric Fields as Future Smart Reagents in Chemistry, Nature Chem. 2016, 8, 1091 (2016).
2 (a) Aragonès, A. C.; Haworth, N. L. ; Darwish, N. ; Ciampi, S. ; Bloomfield, N. J. ; Wallace, G. G. ; Diez-Perez, I. ; Coote, M.L. Electrostatic catalysis of a Diels–Alder reaction, Nature, 2016, 531, 88– 91; (b) The use of electric fields to catalyse chemical reactions is in principle scalable. See: Lin, Z.; Zeng, X.; Yu, S. Enhancement of Ethanol-Acetic Acid Esterification Under Room Temperature and Non-Catalytic Condition via Pulsed Electric Field Application. Food Bioprocess Technol. 2012, 5, 2637-2645
3 Wang, Z.; Danovich, D.; Ramanan, R.; Shaik, S. Oriented-External Electric Fields Create Absolute Enantioselectivity in Diels-Alder Reactions: Importance of the Molecular Dipole Moment. J. Am. Chem. Soc. 2018, 140, 13350-13359.
4 See a recent feature article by J. Howgego [a feature editor at New Scientist]: Field of Influence, Chemistry World, 2018, 22 January 2018, 1-9.
5 For a tutorial, see: Shaik, S.; Ramanan, R.; Danovich, D.; Mandal, D. Structure and Reactivity/Selectivity Control by Oriented External Electric Fields. Chem. Soc. Rev. Tutorial, 2018, 47, 5125-5145.

Tuesday 1 October 2019 at 4.00 P.M.

COFFEE AND TEA WILL BE SERVED AT 3.45 P.M.

!!VENUE TO BE CONFIRMED!!
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