# AIMMS publication report for: 2020-10-26

1. Scientific Perspectivism in Secondary-School Chemistry Educa (2020-8)
2. Current Trends in Dynamical Systems in Biology and Natural S (2020-5)
3. Origin of rate enhancement and asynchronicity in iminium cat (2020-8)
4. Kohn-Sham equations with functionals from the strictly-corre (2020-8)
5. Folding Assessment of Incorporation of Noncanonical Amino Ac (2020-9)
6. Innovation in pharmaceutical R&D: mapping the research lands (2020-10)
7. *N-Heterocyclic Silylenes as Ligands in Transition Metal Carb (2020-9)*
8. *Understanding the 1,3-Dipolar Cycloadditions of Allenes (2020-9)*
9. *Environmental Effects with Frozen-Density Embedding in Real- (2020-9)*
10. *Light-Matter Hybrid-Orbital-Based First-Principles Methods: (2020-9)*
11. *Neutralizing effects of small molecule inhibitors and metal (2020-9)*
12. *Living with breakthrough: Two-dimensional liquid-chromatogra (2020-9)*
13. *Effect of Alkali Metal Cations on Length and Strength of Hyd (2020-9)*
14. *Scientific Perspectivism in Secondary-School Chemistry Educa (2020-10)*
15. *Neurobehavioral effects of cyanobacterial biomass field extr (2020-9)*
16. *The atypical chemokine receptor 3 interacts with Connexin 43 (2020-9)*

### 1) Scientific Perspectivism in Secondary-School Chemistry Education: Integrating Concepts and Skills in Chemical Thinking

* Landa, I., Westbroek, H., Janssen, F., van Muijlwijk-Koezen, J. E., Meeter, M.
* LEARN! - Learning sciences, Team Secondary Education, Innovations in Human Health & Life Sciences, AIMMS, Educational and Family Studies, ICLON, Leiden University
* Science & Education
* https://doi.org/https://doi.org/10.1007/s11191-020-00145-3
* Corresponding author: Westbroek, H.
* Published 7 Aug 2020 (early online None)
* Processed: 2020-8

The importance of learning chemical ways of thinking is widely recognized. Various frameworks have been developed to address the essence of chemistry and chemical thinking. However, very few studies have focused on how chemical ways of thinking can be defined. To elaborate chemical ways of thinking, this paper draws on scientific perspectivism (Giere 2010; Wimsatt 2007; Thagard 2012). Scientific perspectivism states that, within each general domain, several broadly accepted theoretical models exist side by side. These general theoretical models, or theoretical perspectives, determine which research questions are generated, which types of models are developed, and which criteria are important for evaluating models. A theoretical perspective can be captured in a core reasoning that embodies the fundamental relationship between model and the “real world.” Starting with their most basic form, perspectives can be used in learning how to reason about all types of ill-structured problems, directing and organizing knowledge development, and integrating knowledge and skills. The study is part of a research project on how perspectivism can be applied to the design of secondary-school chemistry education. This particular study concerns the identification, elaboration, and validation of four chemical perspectives for secondary-school chemistry education. We use these perspectives to indicate the consequences of taking a perspectivism approach to a curriculum framework. We conclude with discussing the consequences for secondary chemistry curriculum.

### 2) Current Trends in Dynamical Systems in Biology and Natural Sciences

* Aguiar, M. (ed.), Braumann, C. (ed.), Kooi, B. (ed.), Pugliese, A. (ed.), Stollenwerk, N. (ed.)
* Molecular Cell Biology, AIMMS, Dipartimento di Matematica, University of Trento, University of Lisbon
* None
* https://doi.org/10.1007/978-3-030-41120-6
* Corresponding author: None
* Published 2020 (early online None)
* Processed: 2020-5

This book disseminates the latest results and envisages new challenges in the application of mathematics to various practical situations in biology, epidemiology, and ecology. It comprises a collection of the main results presented at the Ninth Edition of the International Workshop “Dynamical Systems Applied to Biology and Natural Sciences – DSABNS”, held from 7 to 9 February 2018 at the Department of Mathematics, University of Turin, Italy. While the principal focus is ecology and epidemiology, the coverage extends even to waste recycling and a genetic application. The topics covered in the 12 peer-reviewed contributions involve such diverse mathematical tools as ordinary and partial differential equations, delay equations, stochastic equations, control, and sensitivity analysis. The book is intended to help both in disseminating the latest results and in envisaging new challenges in the application of mathematics to various practical situations in biology, epidemiology, and ecology.

### 3) Origin of rate enhancement and asynchronicity in iminium catalyzed Diels-Alder reactions

* Vermeeren, P., Hamlin, T. A., Fernández, I., Bickelhaupt, F. M.
* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, Complutense University
* Chemical Science
* https://doi.org/10.1039/d0sc02901g
* Corresponding author: Hamlin, T. A.
* Published 21 Aug 2020 (early online 9 Jul 2020)
* Processed: 2020-8

The Diels-Alder reactions between cyclopentadiene and various α,β-unsaturated aldehyde, imine, and iminium dienophiles were quantum chemically studied using a combined density functional theory and coupled-cluster theory approach. Simple iminium catalysts accelerate the Diels-Alder reactions by lowering the reaction barrier up to 20 kcal mol-1 compared to the parent aldehyde and imine reactions. Our detailed activation strain and Kohn-Sham molecular orbital analyses reveal that the iminium catalysts enhance the reactivity by reducing the steric (Pauli) repulsion between the diene and dienophile, which originates from both a more asynchronous reaction mode and a more significant polarization of the π-system away from the incoming diene compared to aldehyde and imine analogs. Notably, we establish that the driving force behind the asynchronicity of the herein studied Diels-Alder reactions is the relief of destabilizing steric (Pauli) repulsion and not the orbital interaction between the terminal carbon of the dienophile and the diene, which is the widely accepted rationale.

### 4) Kohn-Sham equations with functionals from the strictly-correlated regime: Investigation with a spectral renormalization method

* Grossi, J., Musslimani, Z. H., Seidl, M., Gori-Giorgi, P.
* Theoretical Chemistry, AIMMS, VU University, Florida State University
* Journal of Physics Condensed Matter
* https://doi.org/10.1088/1361-648X/abace2
* Corresponding author: Gori-Giorgi, P.
* Published 11 Nov 2020 (early online 27 Aug 2020)
* Processed: 2020-8

We re-adapt a spectral renormalization method, introduced in nonlinear optics, to solve the Kohn-Sham (KS) equations of density functional theory, with a focus on functionals based on the strictly-correlated electrons (SCE) regime, which are particularly challenging to converge. Important aspects of the method are: (i) the eigenvalues and the density are computed simultaneously; (ii) it converges using randomized initial guesses; (iii) easy to implement. Using this method we could converge for the first time the Kohn-Sham equations with functionals that include the next leading term in the strong-interaction limit of density functional theory, the so called zero-point energy (ZPE) functional as well as with an interaction-strength-interpolation functional that includes both the exact SCE and ZPE terms. This work is the first building block for future studies on quantum systems confined in low dimensions with different statistics and long-range repulsions, such as localization properties of fermions and bosons with strong long-range repulsive interactions in the presence of a random external potential.

### 5) Folding Assessment of Incorporation of Noncanonical Amino Acids Facilitates Expansion of Functional-Group Diversity for Enzyme Engineering

* Drienovská, I., Gajdoš, M., Kindler, A., Takhtehchian, M., Darnhofer, B., Birner-Gruenberger, R., Dörr, M., Bornscheuer, U. T., Kourist, R.
* Organic Chemistry, AIMMS, Graz University of Technology, Medical University of Graz, BioTechMed-Graz, Vienna University of Technology, University of Greifswald
* Chemistry - A European Journal
* https://doi.org/10.1002/chem.202002077
* Corresponding author: Kourist, R.
* Published 25 Sep 2020 (early online None)
* Processed: 2020-9

Protein design is limited by the diversity of functional groups provided by the canonical protein „building blocks“. Incorporating noncanonical amino acids (ncAAs) into enzymes enables a dramatic expansion of their catalytic features. For this, quick identification of fully translated and correctly folded variants is decisive. Herein, we report the engineering of the enantioselectivity of an esterase utilizing several ncAAs. Key for the identification of active and soluble protein variants was the use of the split-GFP method, which is crucial as it allows simple determination of the expression levels of enzyme variants with ncAA incorporations by fluorescence. Several identified variants led to improved enantioselectivity or even inverted enantiopreference in the kinetic resolution of ethyl 3-phenylbutyrate.

### 6) Innovation in pharmaceutical R&D: mapping the research landscape

* Romasanta, A. K., van der Sijde, P., van Muijlwijk-Koezen, J. E.
* Innovations in Human Health & Life Sciences, AIMMS, Organization & Processes of Organizing in Society (OPOS), Network Institute, Organization Sciences
* None
* https://doi.org/https://doi.org/10.1007/s11192-020-03707-y
* Corresponding author: Romasanta, A. K.
* Published 10 Oct 2020 (early online None)
* Processed: 2020-10

In response to the increasing number and breadth of innovation studies on the pharmaceutical industry, we mapped the literature to show the trends in recent research and to indicate areas for further research. In the first phase, we analyzed articles on the pharmaceutical industry published in innovation journals. We used these articles’ textual and citation data and applied hybrid cluster analysis. Three main clusters were produced based on the level of analysis innovation scholars had used to investigate the industry: macro, meso and micro. We describe the research topics within these clusters and show that, overall, innovation scholars increasingly focus on the meso-level, analyzing the relationships across different firms. This shift in interest toward the collaborative nature of drug discovery and development was also apparent in macro- and micro-level studies. To explore how this literature is used by scientists in the industry, our second phase involved analysis of the citing articles published in pharmaceutical journals. Using our findings, we propose research areas that can be further explored in order to create an engaged and better-integrated literature on pharmaceutical innovation.

### *7) N-Heterocyclic Silylenes as Ligands in Transition Metal Carbonyl Chemistry: Nature of Their Bonding and Supposed Innocence*

* Krahfuß, M. J., Nitsch, J., Bickelhaupt, F. M., Marder, T. B., Radius, U.
* Chemistry and Pharmaceutical Sciences, AIMMS, University of Würzburg, VU Amsterdam, University of Würzburg
* Chemistry - A European Journal
* https://doi.org/10.1002/chem.202001062
* Corresponding author: Radius, U.
* Published 1 Sep 2020 (early online 31 Mar 2020)
* Processed: 2020-9

A study on the reactivity of the N-heterocyclic silylene Dipp2NHSi (1,3-bis(diisopropylphenyl)-1,3-diaza-2-silacyclopent-4-en-2-yliden) with the transition metal complexes [Ni(CO)4], [M(CO)6] (M=Cr, M ...

### *8) Understanding the 1,3-Dipolar Cycloadditions of Allenes*

* Yu, S., Vermeeren, P., van Dommelen, K., Bickelhaupt, F. M., Hamlin, T. A.
* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, VU University
* Chemistry - A European Journal
* https://doi.org/10.1002/chem.202000857
* Corresponding author: Bickelhaupt, F. M.
* Published 4 Sep 2020 (early online 27 Mar 2020)
* Processed: 2020-9

We have quantum chemically studied the reactivity, site-, and regioselectivity of the 1,3-dipolar cycloaddition between methyl azide and various allenes, including the archetypal allene propadiene, he ...

### *9) Environmental Effects with Frozen-Density Embedding in Real-Time Time-Dependent Density Functional Theory Using Localized Basis Functions*

* De Santis, M., Belpassi, L., Jacob, C. R., Severo Pereira Gomes, A., Tarantelli, F., Visscher, L., Storchi, L.
* Theoretical Chemistry, AIMMS, University of Perugia, Technical University of Braunschweig, Universite de Lille 2, Gabriele d’Annunzio University
* Journal of chemical theory and computation
* https://doi.org/10.1021/acs.jctc.0c00603
* Corresponding author: None
* Published 8 Sep 2020 (early online 27 Jul 2020)
* Processed: 2020-9

Frozen-density embedding (FDE) represents a versatile embedding scheme to describe the environmental effect on electron dynamics in molecular systems. The extension of the general theory of FDE to the ...

### *10) Light-Matter Hybrid-Orbital-Based First-Principles Methods: The Influence of Polariton Statistics*

* Buchholz, F., Theophilou, I., Giesbertz, K. J., Ruggenthaler, M., Rubio, A.
* Theoretical Chemistry, AIMMS, Max Planck Institute for the Structure and Dynamics of Matter, Simons Foundation
* Journal of chemical theory and computation
* https://doi.org/10.1021/acs.jctc.0c00469
* Corresponding author: None
* Published 8 Sep 2020 (early online 21 Jul 2020)
* Processed: 2020-9

A detailed understanding of strong matter-photon interactions requires first-principle methods that can solve the fundamental Pauli-Fierz Hamiltonian of nonrelativistic quantum electrodynamics efficie ...

### *11) Neutralizing effects of small molecule inhibitors and metal chelators on coagulopathic Viperinae snake venom toxins*

* Xie, C., Albulescu, L. O., Bittenbinder, M. A., Somsen, G. W., Vonk, F. J., Casewell, N. R., Kool, J.
* AIMMS, BioAnalytical Chemistry, Liverpool School of Tropical Medicine, VU University, Centre for Analytical Sciences Amsterdam (CASA), Naturalis Biodiversity Center
* Biomedicines
* https://doi.org/10.3390/BIOMEDICINES8090297
* Corresponding author: Kool, J.
* Published Sep 2020 (early online 20 Aug 2020)
* Processed: 2020-9

Animal-derived antivenoms are the only specific therapies currently available for the treatment of snake envenoming, but these products have a number of limitations associated with their efficacy, saf ...

### *12) Living with breakthrough: Two-dimensional liquid-chromatography separations of a water-soluble synthetically grafted bio-polymer*

* van de Ven, H. C., Purmova, J., Groeneveld, G., Bos, T. S., Gargano, A. F., van der Wal, S., Mengerink, Y., Schoenmakers, P. J.
* BioAnalytical Chemistry, AIMMS, Nouryon Chemicals, University of Amsterdam, DSM Food Specialties
* Separations
* https://doi.org/10.3390/separations7030041
* Corresponding author: van de Ven, H. C.
* Published Sep 2020 (early online 15 Jul 2020)
* Processed: 2020-9

In this study, we evaluate the use of various two-dimensional liquid chromatographic methods to characterize water-soluble, synthetically grafted bio-polymers, consisting of long poly(acrylic acid) ch ...

### *13) Effect of Alkali Metal Cations on Length and Strength of Hydrogen Bonds in DNA Base Pairs*

* Stasyuk, O. A., Solà, M., Swart, M., Fonseca Guerra, C., Krygowski, T. M., Szatylowicz, H.
* AIMMS, Theoretical Chemistry, University of Girona, ICREA, University of Warsaw, Warsaw University of Technology
* ChemPhysChem
* https://doi.org/10.1002/cphc.202000434
* Corresponding author: Stasyuk, O. A.
* Published 15 Sep 2020 (early online 9 Jul 2020)
* Processed: 2020-9

For many years, non-covalently bonded complexes of nucleobases have attracted considerable interest. However, there is a lack of information about the nature of hydrogen bonding between nucleobases wh ...

### *14) Scientific Perspectivism in Secondary-School Chemistry Education: Integrating Concepts and Skills in Chemical Thinking*

* Landa, I., Westbroek, H., Janssen, F., van Muijlwijk, J., Meeter, M.
* Team Secondary Education, LEARN! - Learning sciences, Innovations in Human Health & Life Sciences, AIMMS, Educational and Family Studies, VU University, Leiden University
* Science and Education
* https://doi.org/10.1007/s11191-020-00145-3
* Corresponding author: Westbroek, H.
* Published 1 Oct 2020 (early online 7 Aug 2020)
* Processed: 2020-10

The importance of learning chemical ways of thinking is widely recognized. Various frameworks have been developed to address the essence of chemistry and chemical thinking. However, very few studies h ...

### *15) Neurobehavioral effects of cyanobacterial biomass field extracts on zebrafish embryos and potential role of retinoids*

* Pípal, M., Legradi, J., Smutná, M., Kočí, T., Priebojová, J., Bláhová, L., Krauss, M., Hilscherová, K.
* E&H: Environmental Health and Toxicology, AIMMS, Masaryk University, Helmholtz Centre for Environmental Research
* Aquatic Toxicology
* https://doi.org/10.1016/j.aquatox.2020.105613
* Corresponding author: Hilscherová, K.
* Published Nov 2020 (early online 6 Sep 2020)
* Processed: 2020-9

Cyanobacteria are known for their ability to produce and release mixtures of up to thousands of compounds into the environment. Recently, the production of novel metabolites, retinoids, was reported f ...

### *16) The atypical chemokine receptor 3 interacts with Connexin 43 inhibiting astrocytic gap junctional intercellular communication*

* Fumagalli, A., Heuninck, J., Pizzoccaro, A., Moutin, E., Koenen, J., Séveno, M., Durroux, T., Junier, M. P., Schlecht-Louf, G., Bachelerie, F., Schütz, D., Stumm, R., Smit, M. J., Guérineau, N. C., Chaumont-Dubel, S., Marin, P.
* Medicinal chemistry, AIMMS, Université de Montpellier, Sorbonne Université, ComUE Paris-Saclay, Friedrich Schiller University Jena
* Nature Communications
* https://doi.org/10.1038/s41467-020-18634-y
* Corresponding author: Marin, P.
* Published 1 Dec 2020 (early online 25 Sep 2020)
* Processed: 2020-9

The atypical chemokine receptor 3 (ACKR3) plays a pivotal role in directing the migration of various cellular populations and its over-expression in tumors promotes cell proliferation and invasiveness ...