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Thierry RANDOUX
Président de la SRC en 2016-2017

Jean-Claude Braekman, secrétaire général de la SRC de 2001 à 2017

Jean-Claude Braekman est né à Bruxelles en 1942. Après ses humanités à l'Athénée de Saint-Gilles, il entame en 1960 des études en sciences chimiques à l'Université libre de Bruxelles et obtient sa licence en 1964 après un mémoire réalisé sous la direction du professeur Jacques Pécher dans le service de chimie organique dirigé à l'époque par le professeur Richard Henri Martin. Il obtiendra en 1968 son titre de docteur en sciences après avoir défendu une thèse intitulée « Contribution à l'étude structurale, spectroscopique et chimique d'alcaloïdes mineurs de *Voacanga Chalotiana* ». C'est en 1981 qu'il obtient l'Agrégation de l'Enseignement Supérieur.

Chargé de recherche au FNRS, en 1971, il rejoindra les laboratoires de chimie organique du professeur D.B. Mc Lean à la Mc Master University à Hamilton, Ontario, Canada où il se familiarisera aux techniques d'étude de la biosynthèse des métabolites secondaires.
Devenu chercheur qualifié au FNRS en 1974, il poursuivra ensuite ses travaux sur l'étude de la défense chimique des insectes et des invertébrés marins au sein du Collectif de Bio-Ecologie de l'UniversitélLibre de Bruxelles créé par les professeurs Bernard Tursch et Jean Bouillon.

Jean-Claude Braekman mènera ses recherches pendant plus de 30 ans, toujours en lien avec la chimie des produits naturels : isolement et détermination de structure de nouveaux métabolites secondaires issus d'insectes et d'invertébrés marins, étude des mécanismes de biosynthèse et synthèse totale d'un grand nombre de ces molécules.

Jean-Claude Braekman est auteur et co-auteur de 206 articles publiés dans des revues internationales mais également de 13 articles de revue, 10 chapitres de livre, 9 compte-rendus de conférence et 5 brevets.

Jean-Claude Braekman sera également un enseignant très actif qui partagera sa passion de la chimie avec les étudiants de candidature et licence (NDLR actuellement intitulés bachelier et master en chimie), mais aussi avec les étudiants bio-ingénieurs.
Il accédera à l'éméritat en 2006.

La chimie est et sera toujours au centre de la vie de Jean-Claude Braekman qui s'est constamment impliqué dans un grand nombre d'associations et organisations scientifiques belges et internationales, mais également dans la promotion et la vulgarisation de la chimie.

Jean-Claude Braekman est une cheville ouvrière de la Société Royale de Chimie. Il en deviendra membre en 1964 et sera successivement secrétaire de la Section de Bruxelles, Président de la Section de Bruxelles, Président de la Division de Chimie Organique,

Secrétaire-Général adjoint et enfin Secrétaire Général. Il occupera ce dernier poste pendant 16, ans de 2001 à 2017.

Infatigable, fidèle et engagé, il permettra à la Société Royale de Chimie de remplir ses missions visant à fédérer tous ceux pour qui la chimie constitue un centre d'intérêt (chercheurs, enseignants, industriels), à favoriser les échanges générateurs d'idées et d'innovation, à promouvoir l'image de la chimie. Un des ses points d'attention tout particuliers sera focalisé sur les jeunes chimistes pour les aider à se rencontrer, à s'intégrer dans la communauté scientifique et industrielle de la chimie.

Nous tenons à remercier très sincèrement Jean-Claude Braekman pour son implication exemplaire, sans faille et sans relâche dans la Société Royale de Chimie.

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Dernières nouvelles des jeunes chimistes

1. Les Jeunes Chimistes ?

La Division des Jeunes Chimistes de la SRC est la division qui se focalise sur les jeunes acteurs de la chimie, qu'ils soient mémorants, doctorants ou post-doctorants. Elle a pour but de promouvoir la rencontre et les échanges entre les jeunes chimistes des différentes universités de la fédération Wallonie-Bruxelles au travers d'activités qui leur sont réservées. La division des jeunes chimistes favorise également le contact entre les chimistes sur le point d'être diplômés et les acteurs du monde industriel belge.

Une équipe de 11 doctorants représentant l'ensemble des universités de la fédération Wallonie-Bruxelles œuvre à l'organisation et l'élaboration des activités des jeunes chimistes. Ces activités, qu'elles soient à caractère scientifique ou convivial, se veulent avant tout des occasions pour les jeunes chimistes de nouer des contacts entre eux afin que le paysage de la chimie de demain soit plus collaboratif que jamais.

Cette année, le comité des jeunes chimistes se renouvelle, et accueille plusieurs nouveaux membres. C'est l'occasion de faire naître des idées pour créer de nouvelles activités. En 2018, les activités traditionnelles des jeunes chimistes ont eu lieu et trois visites d'entreprises ont été réalisées.

2. La journée rencontre 2018

Notre événement phare est la Journée-Rencontre, puisqu'elle rassemble les jeunes chercheurs lors d'une journée de conférences multidisciplinaires organisée annuellement. Cette journée de conférences unique en son genre a la particularité de n'accueillir parmi ses participants, actifs ou spectateurs, que des mémorants, doctorants ou post-doctorants. Cela permet à ces jeunes chercheurs de présenter leurs résultats dans une atmosphère plus sereine et moins intimidante que celle d'un congrès de plus grande ampleur. Les communications orales ou par poster sont proposées et doivent être réalisées en anglais. Cette activité est soutenue par l'école doctorale thématique EDT CHIM et est donc valorisable pour la formation doctorale des participants. Cette journée constitue une opportunité idéale pour les jeunes de s'exercer à la communication scientifique et à la vulgarisation dans un cadre amical et convivial. À chaque édition de cette journée, le meilleur poster ainsi que la meilleure communication orale sont récompensés par des prix. Ces prix sont décernés par l'ensemble des participants à la journée rencontre pour les communications les plus efficaces de la journée. La remise des prix est suivie par un traditionnel verre de l'amitié, occasion pour les participants de se réconforter et d'éventuellement approfondir les questions évoquées durant la journée.

Figure 1: Photo de groupe des participants à la journée rencontre des jeunes chimistes 2018.

L'édition 2018 de la journée rencontre a eu la particularité d'accueillir la première édition du concours Jean-Claude Braekman. Ce concours éponyme met à l'honneur le secrétaire général émérite de la SRC pour ses 17 années de service à la Société Royale de Chimie. Le concours lui-même a pour vocation de promouvoir la mobilité des jeunes chercheurs dans le monde. Il récompense le doctorant ayant donné la meilleure présentation de courte durée (5min) au sujet d'une collaboration avec un laboratoire étranger qui a donné lieu à un voyage. Ce prix d'une valeur de 500€est remis par un jury constitué de membres du comité directeur de la SRC, sur base de la clarté de la présentation et de l'importance de la collaboration dans le travail accompli. Tous les membres du comité de la division des Jeunes Chimistes en profitent pour remercier chaleureusement la SRC pour son soutien.

Lors de la 11ème édition, organisée à l'Université Catholique de Louvain le 30 mars 2018, 29 étudiants provenant des 5 universités francophones belges (UCL, ULB, UNamur, ULiège et UMons) se sont rencontrés. 11 communications orales ont été données lors de cette journée, et 14 posters ont été présentés. Le prix de la meilleure communication orale, d'une valeur de 200€, a été décerné à Luc Jacobs (ULB) pour sa présentation intitulée «*Surface reactivity of Au-Ag alloys during N_2O+H_2 reactions studied by field emission techniques*».
Le prix Jean-Claude Braekman a, quant à lui, été décerné à Floriane Devaux (ULiège) pour nous avoir présenté sa collaboration avec le laboratoire de chimie biomimétique supramoléculaire du groupe Ivan Huc à l'université de Bordeaux. Durant son séjour à Bordeaux, Floriane a travaillé à la synthèse des composés qu'elle a ensuite caractérisés au laboratoire de Nanochimie de l'Université de Liège.

3. Le tournoi de badminton interuniversitaire

La division des Jeunes Chimistes organise également un tournoi de badminton sur base annuelle, qui rassemble des chercheurs ou non-chercheurs de tout âge provenant de l'ensemble des universités francophones. C'est un moment privilégié pour chacun de faire la rencontre de membres d'autres universités dans une atmosphère conviviale et sportive. L'édition 2018 a eu lieu au complexe Blocry de l'UCL, lors de laquelle 12 équipes se sont affrontées pour la première place tant convoitée. L'équipe « Les tueuses montoises » a finalement remporté le tournoi après que les matchs aient été disputés avec un fairplay notable. Le drink suivant le tournoi a permis aux participants de discuter et de débattre de leurs exploits.

Figure 2: Photo des lauréats des prix remis lors de la journée rencontre des jeunes chimistes. Floriane Devaux (à Gauche, prix Jean-Claude Braekman) et Luc Jacobs (à droite, prix de la meilleure présentation)

4. Visites d'entreprises

Chaque année, plusieurs visites d'entreprise sont organisées par notre division. Celles-ci constituent une occasion pour les étudiants de se renseigner sur les activités des entreprises belges et de rencontrer les acteurs industriels de la chimie en Belgique qui sont de futurs employeurs potentiels.
Cette année, nous avons eu la joie de visiter GSK, INEOS et CENEXI qui nous ont réservé un très bel accueil. Accompagnés d'une vingtaine de participants, nous avons visité l'implantation de Wavre de GSK, et en particulier, la ligne de production de leurs vaccins. L'équipe de GSK nous a donné une présentation générale sur les enjeux de la vaccination dans le monde ainsi que sur le processus de développement et de production des vaccins.
Nous avons été reçus sur l'implantation du campus Solvay de INEOS (R&D) par notre ancienne présidente, Audrey Richard. Cette visite était plus qu'une visite de courtoisie puisqu'elle nous a permis d'en apprendre plus sur cette entreprise méconnue du grand public. INEOS se spécialise dans la fabrication de polyoléfines à destination des industriels. Nous avons pu visiter les différents laboratoires de recherche et de contrôle qualité d'INEOS.

Enfin, l'entreprise CENEXI nous a accueillis sur son site de production à Braine-l'Alleud. Cette entreprise produit des récipients spécifiques destinés au domaine biomédical, tels que des seringues pré-remplies, des ampoules ou des flacons stériles d'oncologie. Lors de cette visite, le personnel de CENEXI nous a d'abord présenté leur entreprise avant de nous montrer leurs zones de production et leurs laboratoires.

5. Le comité se renouvelle

Avec la nouvelle année académique arrive son lot de changements. Notre comité a l'immense regret de voir partir Sébastien Leloux (UCL), Julien Delbrouck (UNamur) et Christophe Frédéric (UNamur) à qui nous souhaitons le meilleur pour la fin de leur thèse ! Mais c'est avec joie que nous accueillons de nouveaux membres : Nadège Marchal, Pauline Tourneur et Maxime Leclercq représentant l'UMons ainsi que Maximilien Richald et Axel Morelle de l'UCL. Maximilien Richald assurera le rôle de vice-président de notre division aux côtés de

Stephan van den Wildenberg cette année. Nicolas Maira conserve son rôle de trésorier ainsi que nos secrétaires Alexia Papageorgiou et Romaric Gérardy.

6. Quoi de neuf pour 2018-2019 ?

Nous vous attendrons bien sûr lors de nos activités traditionnelles, aux alentours de mars 2019, pour la journée rencontre des Jeunes Chimistes et lors de notre tournoi de badminton de juin 2019. Cette année encore, plusieurs visites d'entreprises sont prévues chez les acteurs industriels de la chimie en Belgique. Nous avons pris contact avec notre équivalent flamand, la « Koninklijke Vlaamse Chemische Vereniging » (KVCV). A terme, nous espérons organiser un événement réunissant nos deux communautés. Nous projetons également l'organisation d'une nouvelle activité centrée sur l'information aux nouveaux futurs doctorants.

7. Contact

Si vous désirez des informations complémentaires sur la division des jeunes chimistes de la SRC, ou si vous désirez vous aussi rejoindre ce comité dynamique constitué de jeunes doctorants, n'hésitez pas à nous contacter à jeune-schimistessrc@gmail.com ou à consulter notre site internet http://jc-src.ulb.be/. Vous pouvez également consulter vos représentants locaux au sein de votre université pour de plus amples informations :

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Emergent properties of the compartmentalised Belousov-Zhabotinsky reaction

Abstract
The Belousov-Zhabotinsky reaction is one of the best known oscillatory reaction and constitutes a model of choice to study the synchronisation of chemical oscillators. In experiments, these micro-oscillators can be micelles, droplets in microfluidic assemblies or catalyst-loaded beads, and the wealth of the patterns found in such systems has drawn much interest in the last decade. Using stochastic simulations, we show that the behaviour of an isolated micro-oscillator also displays emergent properties. More generally, we highlight the existence of emergent phenomena that could be generic to oscillatory systems subjected to fluctuations.

Keywords
nonlinear chemistry, oscillations, micro-oscillator, fluctuations

1. Introduction

When a chemical reaction takes place in a closed system, the concentrations of the reactants and products evolve towards equilibrium concentrations. However, if the system is maintained far from thermodynamic equilibrium by the external supply of reactants or the elimination of products, more complex behaviours can arise. In particular, when the chemical mechanism involves feedbacks like autocatalysis, the differential equations describing the evolution of the concentrations in the course of time include nonlinear terms [1]. To name a few, oscillations, multistability and chaos are typical phenomena generated by nonlinear chemical reactions maintained out of equilibrium. If the chemical dynamics is further coupled to transport phenomena like diffusion or convection, spatiotemporal patterns can also develop [1].

The Belousov-Zhabotinsky (BZ) reaction constitutes one of the first experimental evidences of the complex dynamics arising from nonlinear chemistry. This reaction was discovered in 1951 by Boris Pavlovich Belousov, who searched for an inorganic analogue of the Krebs cycle. Many other chemical systems including catalytic surface reactions and electrochemical reactions have been shown to generate nonlinear behaviours, but the BZ reaction tends to remain the oscillatory reaction *par excellence*. The BZ reaction has been extensively studied both experimentally and theoretically, in many different setups including stirred batch reactors, gel reactors, membranes, populations of catalyst-loaded beads, reverse (water-in-oil) microemulsions and microfluidic assemblies (BZ droplets) [2–4]. Moreover, a photosensitive version of the reaction has been widely exploited to investigate the effects of illumination on nonlinear dynamics [5]. In this work, we focus more specifically on the emergent properties of BZ microemulsions, which are described in more detail in the next section.

2. The Belousov-Zhabotinsky reaction in microemulsion

In BZ droplets and BZ microemulsions, the reactants are confined in the aqueous phase, which is dispersed into a continuous, hydrophobic phase. The majority of the BZ reactants are polar species that tend to be confined in the aqueous phase. However, some nonpolar intermediates are also involved in the reaction and are likely to move to the surfactant layer or the hydrophobic phase, where they can diffuse and eventually enter another micelle or droplet. A collision-coalescence-redispersion mechanism specific to microemulsions [6] further ensures mass exchange between the micelles. These systems display a variety of spatiotemporal patterns that are not present in the "bulk" case, as shown in Figure 1.

While mass transport is crucial to the emergence of new patterns in the BZ microemulsions, the role of other compartmentalisation effects like fluctuations remains unclear. In such configurations, the volume in which the BZ reactants are encapsulated is very small and a given micelle only contains a few tens of molecules of the most abundant species. As a result, large fluctuations in the chemical composition of the micelles are to be expected. The extent to which these intrinsic fluctuations perturb the dynamics of this reaction is still poorly understood. In this context, we have analysed the chemical behaviour of an isolated BZ droplet, in the presence and in the absence of fluctuations. More precisely, we compared the behaviour of a single droplet, subjected to fluctuations, to the dynamics of a corresponding bulk system of macroscopic size, where such fluctuations are not observable. We focused on the impact of fluctuations on the photosensitive version of the reaction and investigated the emergence of fluctuation-induced behaviours.

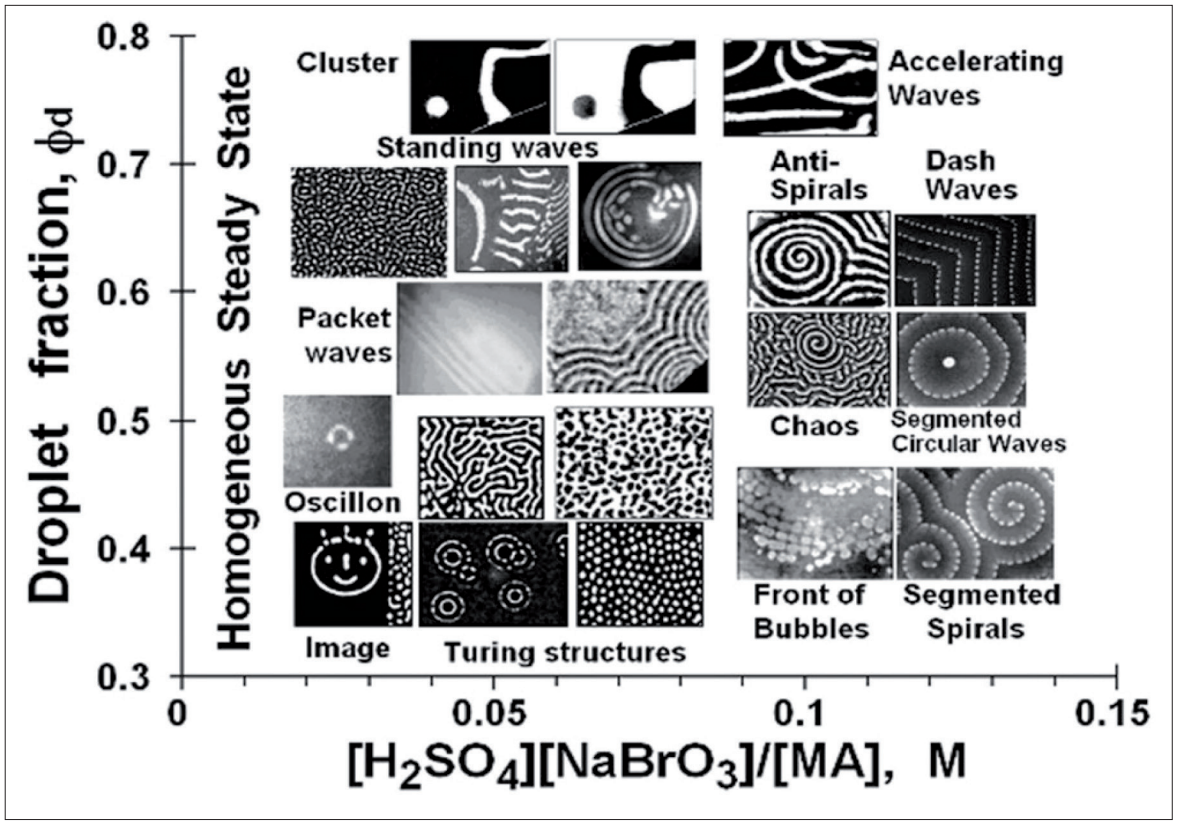

Figure 1: Phase diagram of the behaviours observed in the BZ microemulsions, with respect to the droplet fraction φ_d (the volume of the dispersed phase, i.e., water and surfactant, divided by the total volume of the system) and the ratio of the concentrations of key species. Figure reproduced from reference [4].

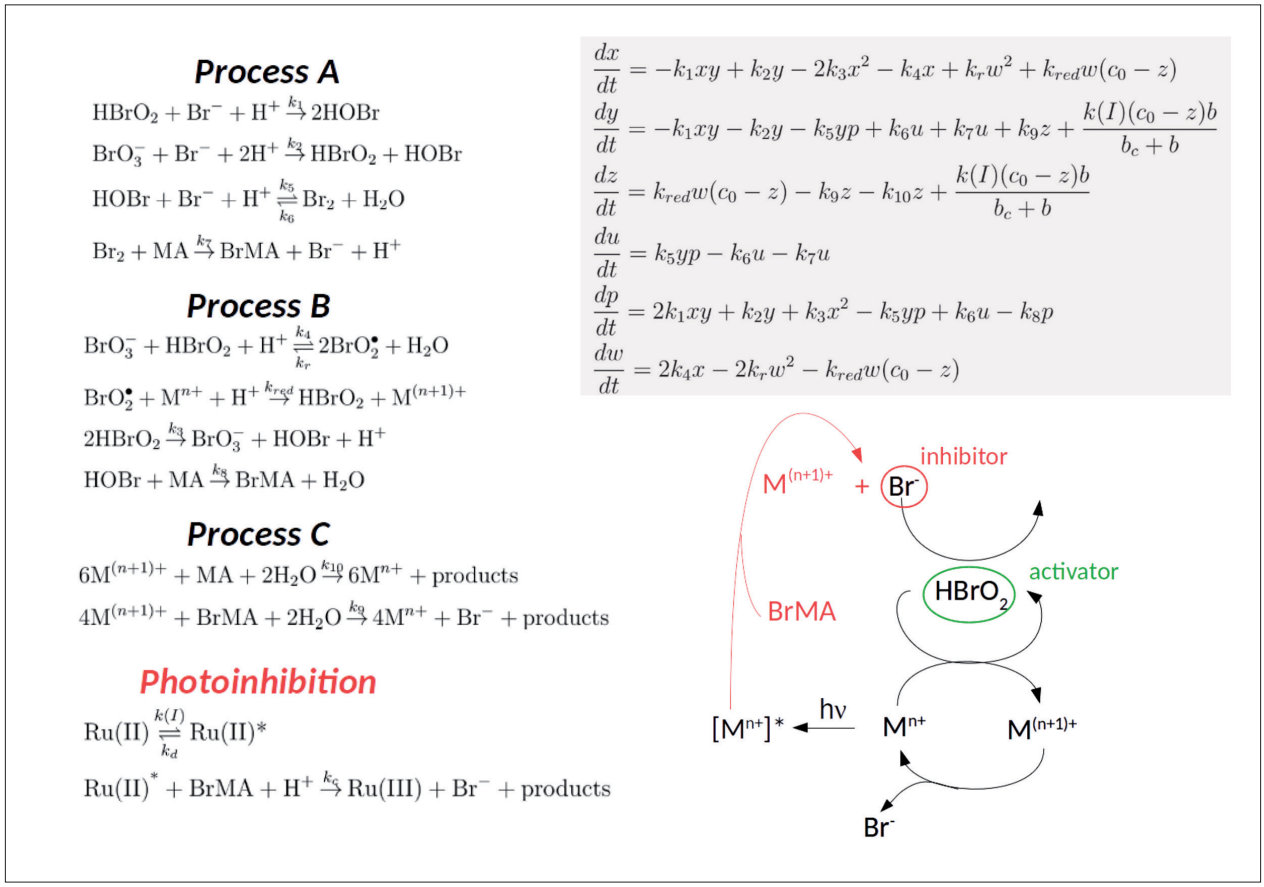

Figure 2: Chemical mechanism of the BZ reaction proposed by Field, Körös and Noyes: (left) chemical equations, (upper right) evolution equations and (lower right) schematic representation of the main feedback loops involved in the mechanism. For clarity, we set the variables x≡[$HBrO_2$], y≡[Br^-], z≡[M^{n+}], u≡[Br_2], p≡[HOBr], w≡[$BrO_2^\bullet$] and the constants c_0≡[M^{n+}]+[$M^{(n+1)+}$], b≡[$BrCH(COOH)_2$]≡[BrMA], b_c≡k_d/k_c, ma≡[$CH_2(COOH)_2$]≡[MA], h≡[H^+] and a≡[BrO_3^-], which have been incorporated in the kinetic constants.

3. Mechanism and model

The first mechanism for the BZ reaction has been proposed by Field, Körös and Noyes in 1972 [7, 8] and many simplified versions of the model (e.g. the Oregonator [9]) have been developed. This mechanism involves bromine, organic and cerium species and can be decomposed in three processes (Figure 2). Bromide (Br^-) and hypobromous acid ($HBrO_2$) were respectively identified as the inhibitor and the activator of the reaction. Typically, the reaction mixture initially contains the catalyst, malonic acid, sulfuric acid and a bromate salt, but small quantities of bromide can also be added to reduce the latency period preceding the appearance of the first oscillation [10].

In Process A, the inhibitor is mainly oxidised by different bromine species. The activator is present in small quantities but is exclusively involved in the oxidation of Br^-. When the inhibitor concentration reaches a critical value, the autocatalysis of the activator becomes the dominant reaction (Process B) and is accompanied by the oxidation of the redox catalyst (M^{n+}). When the reduced form of the catalyst is almost depleted, the autocatalysis stops. Organic species then "reset the clock" in Process C by regenerating the reduced catalyst as well as bromide, which is a key step for the sustainability of the oscillations. Process A can thus start again when the accumulation of bromide is sufficient.

An alternative version of the reaction, which is catalysed by the tris(2,2′-bipyridine)ruthenium(II) complex ($Ru(bpy)_3^{2+}$), displays photosensitive properties [5, 11]. More specifically, the photoinhibition of the oscillations is frequently exploited in systems of BZ beads or BZ droplets

to control the behaviour of the system [3, 4, 10]. The illumination of the system triggers the formation of an excited form of the catalyst, which reacts with an organic species to generate the inhibitor [11]. The combination of the Field-Körös-Noyes (FKN) and the photoinhibition mechanisms yields a model (see Figure 2) that was shown to efficiently reproduce the dynamics of BZ droplets in microfluidic assemblies for appropriate values of the parameters [10]. We investigated the impact of fluctuations on the chemical dynamics of the photosensitive Belousov-Zhabotinsky reaction on the basis of this model.

4. Fluctuation effects on the dynamics of BZ microreactors

4.1. Behaviour of large and ideal systems

The model presented in Figure 2 describes the evolution of the concentrations in an ideal and macroscopic system, *i.e.,* in the absence of fluctuations. Numerical integrations of these equations have shown that the BZ reaction can be at the source of a multitude of nonlinear behaviours ranging from oscillations to birhythmicity and chaos [12]. In the simplest case, the system undergoes transitions, often referred to as *bifurcations* in nonlinear systems, from a stationary state to oscillations, then from oscillations to another stationary state, as one of the control parameters is changed (Figure 3a). This is what happens when the reaction takes place in the dark or under illumination with low light intensity. However, if the system is exposed to higher light intensities, oscillations can coexist with the stationary state (Figure 3b).

4.2. Stochastic simulations

To simulate the fluctuating dynamics of the FKN model, we used stochastic simulations that predict the behaviour of the system as a function of the probability associated to each reactive event [13]. This probability directly depends on the size of the system, *i.e.,* on the volume of the droplet. At each iteration, the reaction probabilities are calculated based on the current state of the system (the number of particles of each species) to define the next reaction to occur and the time that will elapse before this reaction. The number of molecules of each species is then adapted, according to the stoichiometry of the selected reaction.

Stochastic simulations showed that fluctuations impact the behaviour of the system in the neighbourhood of the bifurcations in two

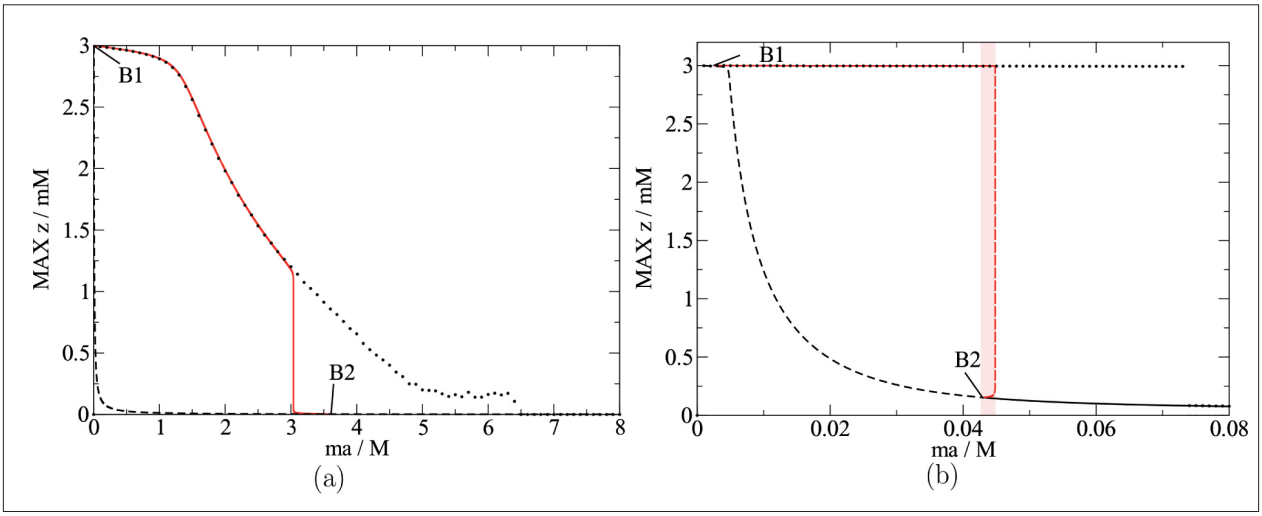

Figure 3: Bifurcation diagrams of z versus ma for (a) low light intensity and (b) high light intensity. The plain lines correspond to stable stationary states and unstable trajectories are represented by dashed lines. The maxima of the oscillations are plotted in red and steady states in black. These results are predicted by the evolution equations shown in Figure 2. The black dots correspond to results of stochastic simulations (maxima of the oscillations or steady states) for $V = 5 \times 10^{-17}$ L. The shaded area corresponds to the domain of coexistence of oscillations and the steady state.

different ways, depending on the light intensity. For low light intensities or in the dark, fluctuations tend to expand the oscillatory domain as indicated by the small dots in Figure 3a. The amplitude of these fluctuation-induced oscillations gradually decreases as the malonic acid concentration is increased, and far from the bifurcation, a noisy stationary state is recovered. The situation is different for high light intensities where oscillations are expected to coexist with a stable steady state for a suitable choice of parameters. In droplets of small volume, large amplitude oscillations exist for a larger range of malonic acid concentration, but in this case, the transition from large amplitude oscillations to the stationary state is much more abrupt (Figure 3b). This difference of behaviour is mainly due to the type of bifurcation leading to oscillations. In both cases, this expansion of the oscillatory domain is particularly relevant for the inhibition of oscillations by light in micro-oscillators. More specifically, our study shows that larger light intensities should be used in small systems to obtain the same efficiency of photoinhibition as in macroscopic systems (Figure 4a).

We further observed that in the domain of coexistence, there is an optimal system size for which the oscillations are more regular than in small and in large systems. This trend can be quantified with the standard deviation of the oscillation period (Figure 4b). For small BZ micro-oscillators, fluctuations induce frequent transitions between the two attractors, which make the oscillations highly irregular, as expected. However, for large systems, the frequency of oscillations also spreads widely. In such cases, the system is characterised by reaction spikes that are separated by periods of latency, during which the system is in the stable stationary state (Figure 4c). This intermittency is due to fluctuations allowing for transitions between the two coexisting regimes, by driving the system beyond the unstable state that separates them (Figure 2b). When the amplitude of the fluctuations is reduced, these

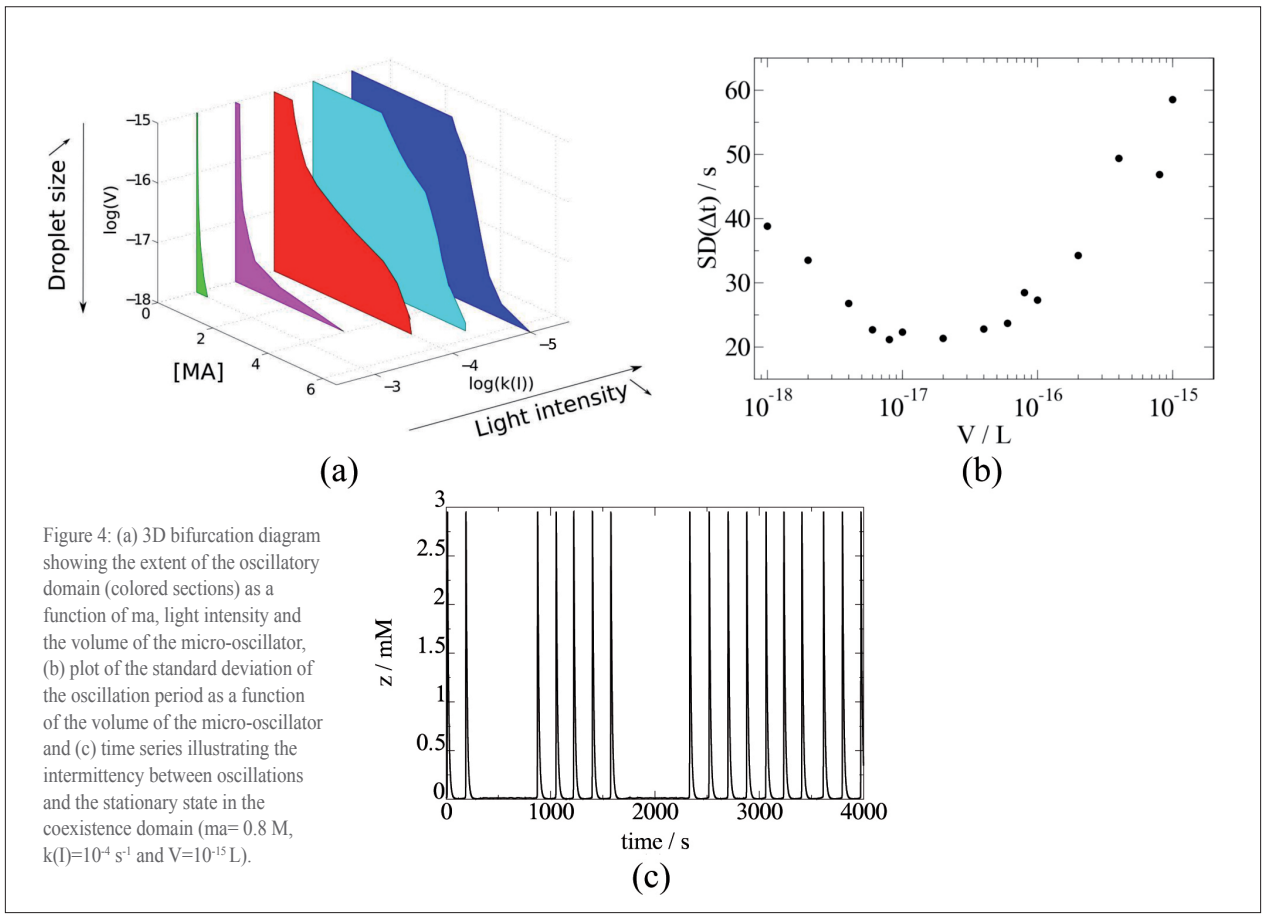

Figure 4: (a) 3D bifurcation diagram showing the extent of the oscillatory domain (colored sections) as a function of ma, light intensity and the volume of the micro-oscillator, (b) plot of the standard deviation of the oscillation period as a function of the volume of the micro-oscillator and (c) time series illustrating the intermittency between oscillations and the stationary state in the coexistence domain (ma= 0.8 M, $k(I)=10^{-4}$ s^{-1} and $V=10^{-15}$ L).

transitions are less frequent, but the "lifetime" of each behaviour increases. For large systems, the dynamics thus consists in long periods of oscillations followed by long phases of latency, and vice-versa.

5. Discussion

To summarise, we investigated the impact of fluctuations of composition on the oscillatory regime displayed by the BZ reaction in the presence and in the absence of photoinhibition. We distinguished two classes of fluctuation-induced phenomena. The first corresponds to the emergence of oscillations sustained by fluctuations in the neighbourhood of bifurcations. This behaviour crucially impacts photoinhibition, which is thus less efficient than in macroscopic systems. However, this property could also be used to tune the behaviour of the system by acting on the size of the system instead of the concentrations or the light intensity. A second fluctuation-induced behaviour takes place inside the oscillatory domain when large-amplitude oscillations coexist with a stable stationary state. In particular, we showed that the effect of noise on the regularity of the period of oscillations can be minimised for a specific droplet size.

Such fluctuation effects have not yet been observed experimentally. On one hand, current experimental studies have focussed on the behaviour of an ensemble of droplets or micelles instead of analysing the dynamics inside an individual compartment. Individual micelles ($V \approx [10^{-21}–10^{-23}]$ L) are moreover not stable outside the microemulsion environment and it is thus not possible to analyse their intrinsic chemical behaviour. On the other hand, our simulations showed that fluctuation effects tend to disappear for droplets with a volume larger than 10^{-12} L, which is the case for the droplets used so far in the microfluidic experiments ($V \approx [5\times10^{-10} - 10^{-9}]$ L).

Nevertheless, the synthesis of droplets of intermediate size ($V \approx [5\times10^{-18}–10^{-12}]$ L), matching the volumes used in our simulations, is technically feasible. Due to the limitations imposed by light microscopy, the detection of the oxidation state of such small droplets should then rely on a change in fluorescence instead of a change in absorbance. In the future, such an experimental setup could be developed to verify the theoretical predictions made *via* the model. More generally, the two fluctuation-induced phenomena identified *via* these simulations could also be exploited to design and control micro-oscillators with specific frequencies.

Acknowledgements

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Opening up new research lines in Lewis acid/base catalysis

Lewis acids and bases play an important role in modern chemistry and are extensively used in academic and industrial laboratories as catalysts, ligands, initiators, scavengers, etc. [1].
In general, *Lewis* acids and *Lewis* bases *combine* and undergo neutralization by forming a Lewis adduct (Figure 1a) [2]. Steric bulk, however, prevents the formation of strong bonds between sterically hindered Lewis acids and bases (Figure 1b) [3].

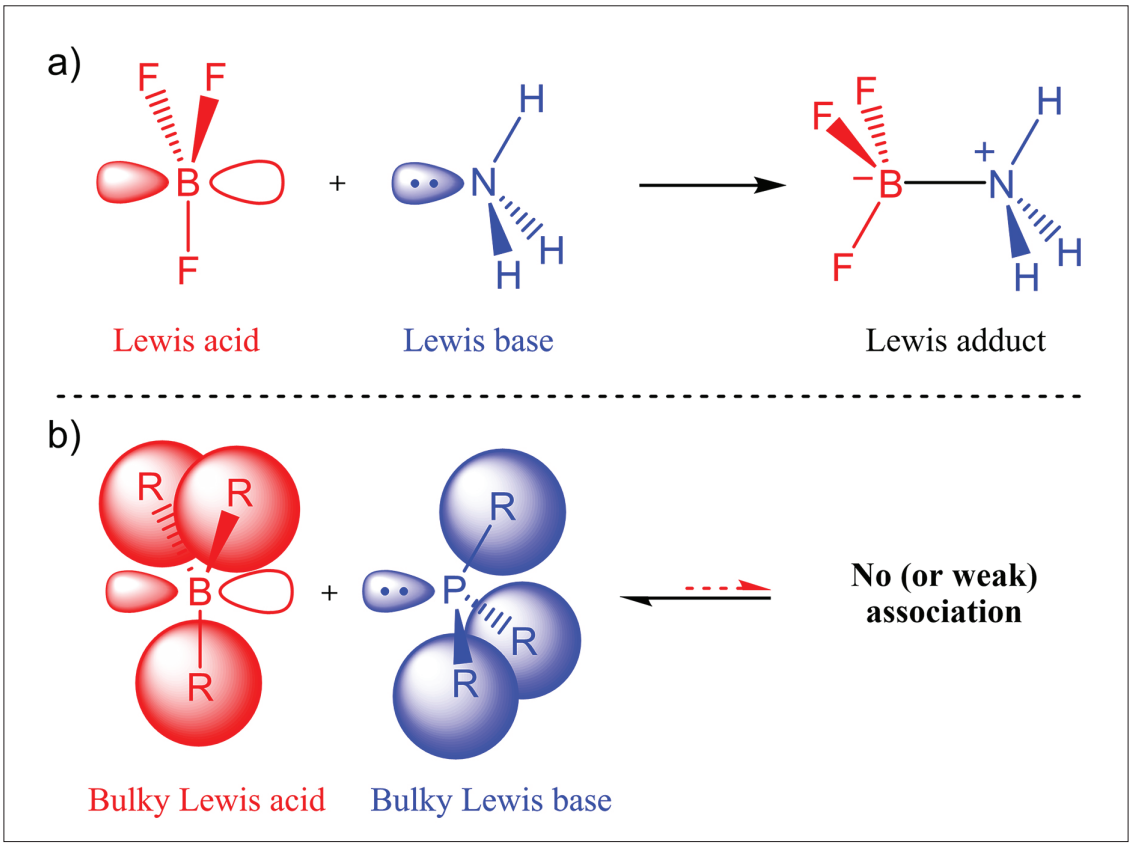

Figure 1: a) Formation of a Lewis acid-base adduct between ammonia and boron trifluoride; b) Schematic representation of an intermolecular frustrated Lewis pair.

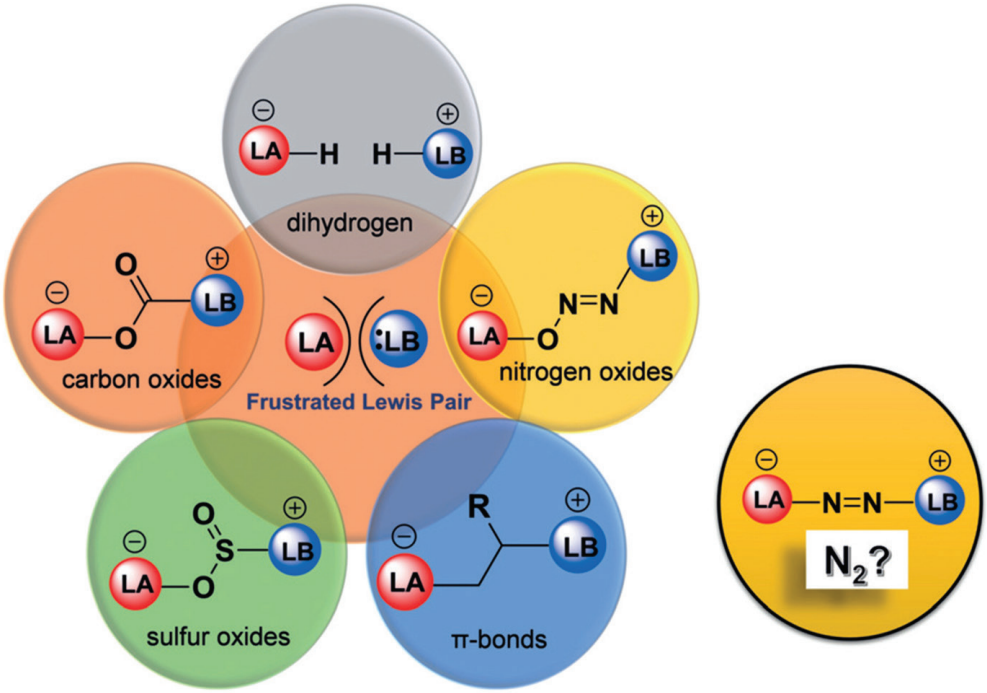

Figure 2: Activation of small molecules with frustrated Lewis pairs. Reproduced from Ref. 4 with permission from John Wiley and Sons.

The resulting frustrated Lewis pairs (FLPs) with unquenched *Lewis* acid/base couples feature an unprecedented potential for cooperative activation of small molecules (H_2, CO_2, SO_2, CO, N_2O) [3].

Fascinated by the latest advances in the field of frustrated Lewis pairs catalysis [4], and with a longstanding interest in kinetic and mechanistic studies, we are interested in examining the fundamental chemistry of activation of small molecules (and of C-H bonds) by new types of Lewis acids and bases [5].
As a rational starting point, we are taking our inspiration from the seminal work of Wittig and Tochtermann on the reactivities of carbon and phosphorus-centred Lewis bases in combination with triphenylborane BPh_3 (Figure 3) [6, 7]. As the C–B and P–B bonds of the Lewis adducts of Ph_3C^- and Ph_3P with the sterically hindered BPh_3 Lewis acids are very weak, dissociation and subsequent reactions with a variety of substrates (ethers, alkenes [6] and 1,2-dehydrobenzene (benzyne) [7]) have been observed.
In sharp contrast, triphenylborane is completely associated with the ring strained triptycyl anion (Figure 4), which is more compact and basic than the trityl anion, and the resulting Lewis adduct is even air and water stable [8]. Triptycyllithium is also spontaneously carbonylated by CO_2 at low temperatures [9].

In view of the intense current interest in the development of sterically hindered Lewis bases [10], we are re-investigating the potential of the triptycyl anion and of the structurally related phospha [11] and aza-triptycenes [12] Lewis bases (Figure 5) as constituent of frustrated Lewis pairs in our research group.

A deep understanding of their reactivities will be obtained by performing NMR and spectrophotometrical binding titrations experiments with a series of Lewis acids of variable sizes and strengths (BF_3, BPh_3, $B(C_6F_5)_3$). Comparison of their stereoelectronic properties (Tolman cone angle θ and electronic parameter [13], pK_a, Lewis basicity…) with those of classical and hindered phosphines will shed light on the potential applications of these triptycene-derived Lewis bases in FLPs catalysis.

These projects are synthetically challenging and expose our graduate and undergraduate students

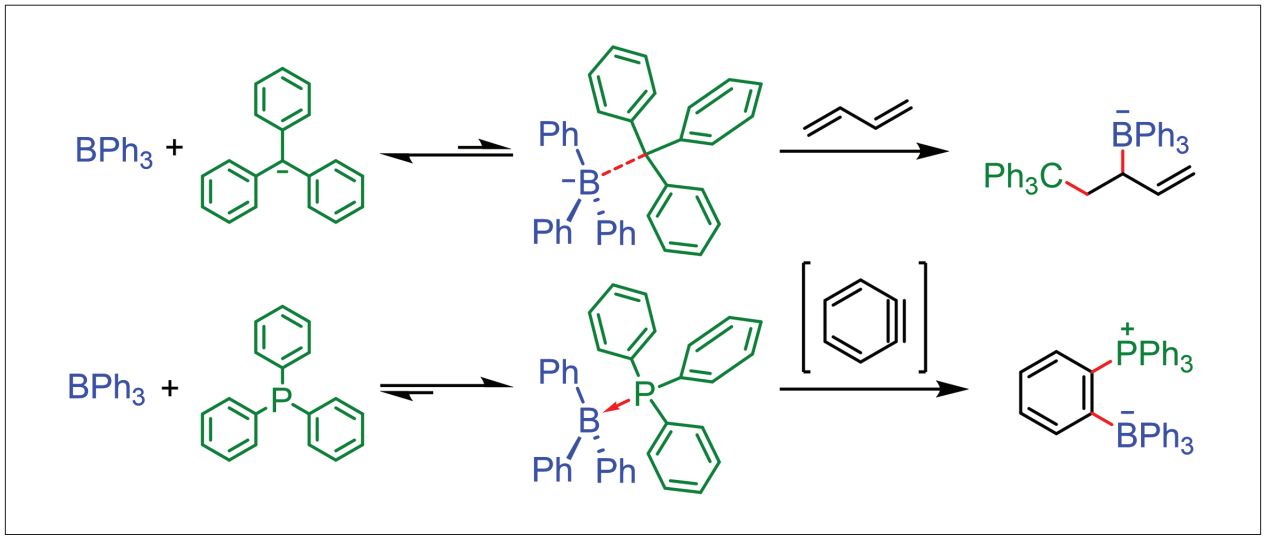

Figure 3: Early examples of reversibly formed Lewis adducts reacting with the π-bonds of 1,3-butadiene (top) and benzyne (bottom) [6, 7].

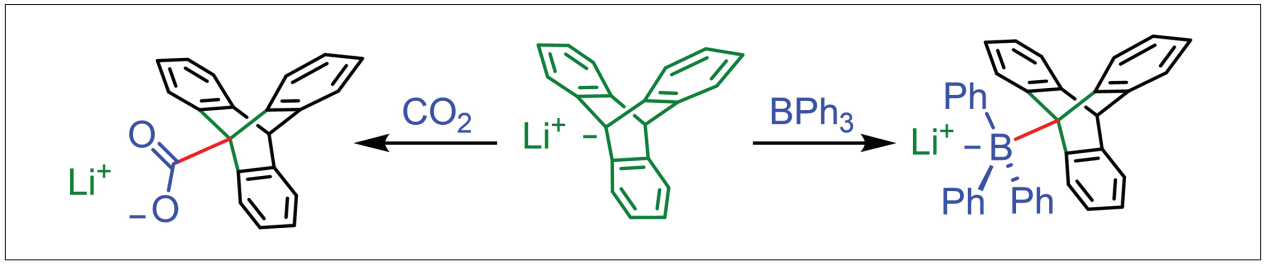

Figure 4: Irreversible association of triptyc-9-yl lithium with CO_2 and BPh_3 [8, 9].

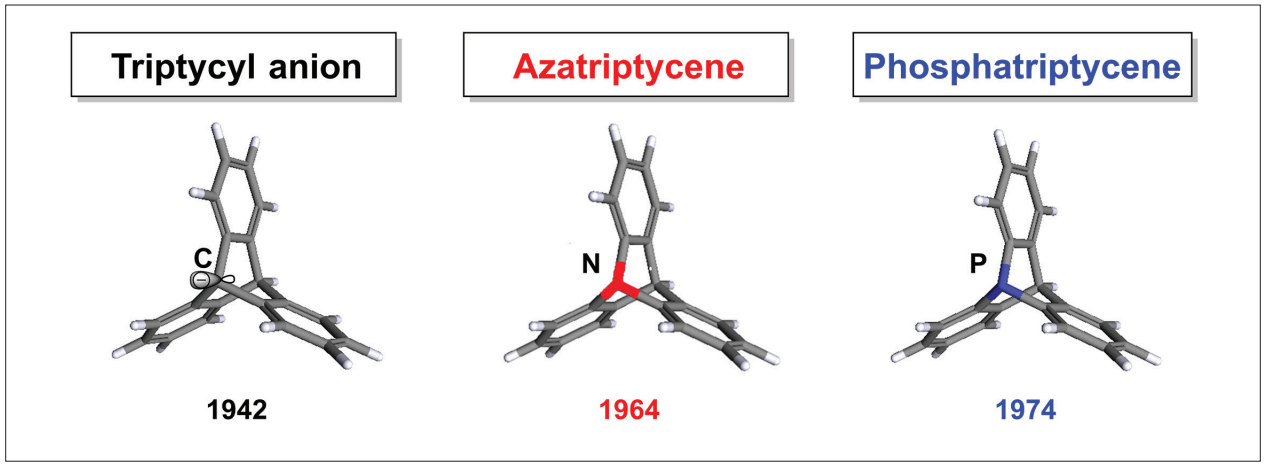

Figure 5: Examples of understudied carbon, nitrogen, and phosphorus Lewis bases.

to a variety of advanced synthetic, spectroscopic, photophysical and computational techniques. For these purposes, we have been developing collaborations with our skilled colleagues in computational chemistry, crystallography, materials and organic chemistry at the University of Namur, and are open to broad scientific discussions with anyone interested in these research areas.

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Author biography

Prof. Guillaume Berionni received his PhD from the University of Versailles (Institut Lavoisier de Versailles) in 2010 for his research on physical organic and supramolecular chemistry under the supervision of Prof. F. Terrier and R. Goumont.

In 2010 he moved to the Ludwig Maximilian University of Munich as a Humboldt postdoctoral fellow under the guidance of Prof. Herbert Mayr and Prof. Paul Knochel. His post-doctoral and subsequent independent research on organometallic and organoboron chemistry has been supported by the Alexander von Humbolt and the DAAD foundations.

Since end 2017 he is Professor of organic chemistry at the University of Namur (Belgium) where he is managing a research team of 3 PhD students, a post-doctoral fellow, a technician and several master students. He is also actively involved in teaching, especially at the master's level. In 2018 he received an incentive grant for scientific research (MIS grant 2018-2020) from the FNRS.

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Repositioning the chemical sciences for a sustainable future


Alain KRIEF


Henning HOPF


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Stephen A. MATLIN

Summary
The chemical sciences face major challenges in the 21st century. Among these, internal challenges include how best to structure the teaching, research, applied interfaces and governance of a mature science in a highly competitive and rapidly changing world. Challenges related to the external environment include how to ensure the relevance of the chemical sciences, how to improve their sometimes tarnished image and reputation, and how to optimise their contribution to solving oncoming global problems. A group of scientists associated with the International Organization for Chemical Sciences in Development has been discussing and writing about these issues for several years and here summarise their published work to date. It is argued that chemistry needs repositioning to achieve its potential in sustainable development. The changes advocated are encapsulated in the concept of 'one-world chemistry'. One implication of this approach is that chemistry needs to embrace systems thinking, partly to improve understanding of the subject itself and partly as a way of developing a wider understanding of the interactions of the chemistry system with other systems. The group has commented on the need for the world of chemistry, including its professional associations at national and international levels, to undertake deep-seated reforms to reorient its thinking and practice. Emphasis has also been placed on the responsibility of individuals and professional associations to adopt and promote the approach of 'scientific temper'; to combat 'fake news'; to reform the deeply flawed word of science publishing which is damaging to the careers of scientists and to the advancement of science; and to give leadership in ensuring equity, diversity and inclusion.

1. Introduction

Chemistry is central to understanding the nature of all matter and to learning how to transform it. While those working in the field are well aware of this, among the public, policy makers, science funders and media there is often much less appreciation of the importance and value of the field. For more than two centuries, chemistry has made outstanding contributions both to the advancement of scientific knowledge and to the creation of products that have been the basis of wealth-generating industries, improved health and enhanced lifestyles [1]. Yet, periodic waves of unpopularity of the field among students and low ratings of the subject and its practitioners and industries among the public have been seen in recent decades – often associated with accidents such as chemical spillages or explosions, with instances of the misuse of chemical substances in warfare or creating drug addiction, or with pollution of the environment.

The International Organization for Chemical Sciences in Development (IOCD) was founded at UNESCO in 1981 and subsequently registered in Belgium as an international non governmental organization. Initially focused on using the chemical sciences to assist in development in low- and middle-income countries through education, research and capacity development of individuals and institutions, in recent years IOCD has directed its attention to the promotion of the chemical sciences as a core scientific discipline and as central to the achievement of sustainable development globally. Since 2014, a group of four scientists affiliated with IOCD has been meeting to discuss and write about these issues. Formalised under the name 'Chemists for Sustainability' (C4S), this IOCD core action group (Figure 1) and occasionally additional guest collaborators has so far produced around 20 articles. These have been published in diverse locations including leading chemistry and science journals, magazines, newspapers and websites, sometimes relayed in languages other than English and aimed at a wide range of audiences from science researchers, educators and administrators to the general public. The C4S group has argued that chemistry as a discipline needs redesign and reform, in order to ensure that it is attractive and productive as a science and relevant to solving 21st century challenges. This review summarises the work to date.

2. Repositioning chemistry for the 21st century

Early writings by the C4S group [2,3] acknowledged chemistry as a great enabler that, for two centuries, has played a key role in conquering diseases, solving energy problems, addressing environmental challenges, and providing discoveries that have underpinned new disciplines and spawned new industries. However, it was also recognised that, to meet the demands of the future, this mature science must expand into new frontiers, a move requiring broad support and necessitating that the public and policy-makers understand its pivotal role in every facet of life. Building trust and confidence, the essential bedrocks for long-term support, requires openly acknowledging not only chemistry's considerable achievements but also the problems and harms that have been caused, whether intentionally or not, by some chemical processes, products and wastes.

Figure 1. IOCD action group 'Chemists for Sustainability' meeting in Hyderabad in 2017. Left to right: Alain Krief, Henning Hopf, Stephen Matlin, Goverdhan Mehta

This early work identified several themes that would be picked up in subsequent articles. One of these was the importance of reforming chemistry education at all levels in order to make chemistry better understood, more relevant to contemporary issues and able to inspire future generation of chemists. A paper presented by a member of the C4S group at the 2016 Gordon Research Conference on 'Chemistry Education as an Agent in Global Progress' took to one of the leading fora of chemistry educators the challenge of achieving a chemistry literacy that is relevant to people's lives [4].

Another issue identified was that many of the field's major national and international associations require sweeping reforms to balance their focus on the professional advancement of their members with an active role in bolstering recognition, respect, and understanding for chemistry from the public. It was recognised that changing this balance would require breaking very long-standing traditions of many of these associations, and would need champions to step forward at both leadership and grassroots levels to press the case for reforms. Furthermore, it was emphasised that industry, as a critical constituent of the chemistry community, should do its part by wholeheartedly embracing ethical rules and practices and engaging in responsible chemicals management and responsible innovation. Industry needed to engage with consumers and have frank conversations with a society that demands transparency and has deep concern about risks. This could be supported by academia, working with industry to clearly explain the science, applications, and impacts and relating these to local contexts.

3. Chemistry for sustainable development

Our planet faces a myriad of substantial challenges in the 21st century and many of these were recognised in the Sustainable Development Goals (SDGs) adopted at a UN summit in September 2015 as part of the UN Agenda for Sustainable Development 2030 [5]. The earlier Millennium Development Goals had focused on particular problems of the world's poorest countries, to help overcome which the richer nations would provide aid. However, the new SDGs embrace a global vision of development for all, building on the core principle of sustainability and with responsibility to be shared by all countries according to their capacities.

The C4S group observed that chemistry can and must make pivotal contributions to help realize the ambitious UN Agenda for Sustainable Development, agenda, by developing the processes, products and monitoring mechanisms that the SDG goals and targets require. However, it cautioned that, to do so optimally, chemistry needs to undergo major changes in its priorities, approaches and practices [6,7]. To achieve chemistry's potential, there could not be business as usual, in education, research or practice and the chemical industry needed to fully embrace green chemistry, ethical rules and practices and engage in responsible innovation [8] and responsible chemicals management. The C4S group concluded that chemistry can re-imagine itself as a champion and driver of sustainable development, transforming its image from often being seen as the source of environmental pollution and degradation to being recognized as a core sustainability science – a key driver of practical, sustainable and ethical solutions to many of the world's greatest challenges in the 21st century. A redesign encompassing chemistry's image, approaches and practices was seen as desirable because the world needs chemistry's best endeavours to avert or mitigate the many global crises that are currently unfolding, and also because it will reinvigorate the entire field of chemistry and transform its appeal as an ethical science worthy of investment and esteem by society.

4. 'One-world chemistry' and systems thinking

The nature of the reforms necessary to reposition chemistry as a sustainability science were encapsulated by the C4S group in the concept of 'one-world chemistry' (OWC). This was presented [9-13] by the C4S group as a new orientation for the discipline.

OWC incorporates a number of basic principles. It emphasises the need for chemistry to be a science for the benefit of society, embracing the understanding that human health, animal health and the environment are all interconnected. It therefore requires developing awareness of how chemical systems interact with many other systems, including the physical, biological, and ecological systems of the planet. It recognizes that the solutions to many fundamental and applied problems traverse geographic and disciplinary boundaries and mandate cross-disciplinary approaches. Furthermore, it insists that chemistry must at all times be practiced in an ethical manner, taking account of the short- and long-term impacts of how it is conducted and of the uses, potential uses, and fates of its products and by-products.

Acting on the consequences of these principles requires embracing the mission of sustainability, the employment of systems thinking in relation to all aspects of the practice of chemistry, strengthening the capacity of chemistry for cross-disciplinary working, and improving the productivity of the interface between academia and industry.

The C4S group has repeatedly stressed the importance of enhancing the capacities of chemists for cross-disciplinary working. In the past, chemistry's evolution as a well-defined and separate academic discipline provided a secure base for research that added to fundamental knowledge and contributed to technological applications in chemical, biotechnology and materials industries. But the practice of science – and, in particular, the interaction between disciplines in order to share ideas, advance fields and tackle complex problems – is changing fundamentally in the globalized world of the 21st century. Cross-disciplinary engagements can take a number of different forms: they can be multidisciplinary (bringing together knowledge and problem-solving approaches from a host of fields that can each contribute, 'side-by-side', to different stages or aspects of problem-solving); interdisciplinary (developing expertise in working across the boundaries between chemistry and other disciplines and transferring methods from one discipline to another); or transdisciplinary (beyond interdisciplinary – which still implies the autonomy of subjects working in cooperation – creating a new synthesis of chemistry and other subjects in which knowledge, methods and solutions are developed holistically: recognizing that valuable knowledge can be found in the spaces between defined disciplines, addressing the complexity of problems and the diversity of perceptions of them). It has been argued [14] that the shift from disciplinary to transdisciplinary research corresponds to a transition from compartmentalized, corrective, problem solving approaches to systemic, preventive ones.

A system is an interconnected set of elements that is coherently organized in a way to achieve a function or purpose [15]. One definition of systems thinking, adapted from the Waters Foundation [16], is that it uses strategies to develop understanding of the interdependent components of dynamic systems. Another way of expressing this is that systems thinking is about seeing and understanding systems as wholes rather than as collections of parts. While little attention had hitherto been given to systems thinking in the chemistry domain, it has been a major factor in the development of other science and technology disciplines, including biology and engineering [17,18]. For chemistry, it offers opportunities not only to enhance learning by adopting a broader view that encourages experiential learning and purposeful reflection, but also to develop understanding of how the chemistry system interacts with the physical, biological and environmental systems in which it is located, as well as with human systems (e.g. economic, political, regulatory and social systems) within which chemistry is practiced and its processes and products used.

5. Systems thinking in chemistry education

Ideally, the development of a capacity for systems thinking should begin early in chemistry education, enabling the learner both to benefit from the broader understanding of the discipline that comes with seeing chemistry itself as a system; and to better appreciate how the chemistry

system interacts with and impacts on the world as a whole.

In collaboration with Peter Mahaffy [19], the C4S group has set out the case for chemistry education to adopt systems thinking and begun examining pathways through which this can be achieved. A proposed framework (Figure 2) places the chemistry learner at the centre, interacting with three nodes or essential elements. The learner systems node explores and describes the processes at work for learners in general, while the chemistry teaching and learning node focuses on features of learning processes applied to the unique challenges of learning chemistry. The earth and societal systems node orients chemistry education toward meeting societal and environmental needs articulated in initiatives such as the SDGs and descriptions of the earth's planetary boundaries. Educational systems to address the interface of chemistry with earth and societal systems include green chemistry and sustainability education, and use tools such as life cycle analysis [20,21].

IOCD is currently collaborating with the International Union for Pure and Applied Chemistry (IUPAC) in a global project to develop learning objectives and strategies for infusing systems thinking into chemistry education, using the framework of the three nodes [22].

6. Reforming the role of chemistry organizations

Chemistry organizations should play a leading, pro-active role in the repositioning of chemistry that is required in the 21st century. The C4S group argues that this necessitates reforms in both national (e.g. chemistry societies) and international (e.g. IUPAC) bodies that represent the interests of the discipline and the profession [23,24].

At the national level there are more than 250 diverse chemistry organisations around the world, about quarter of which are national chemistry societies that have traditionally functioned in multiple roles, including as learned societies, voices of the chemistry profession and protectors of the interests of professionals and the public. In a changing environment, not all these bodies have responded effectively to the emerging challenges, such as sustainability, the need to develop

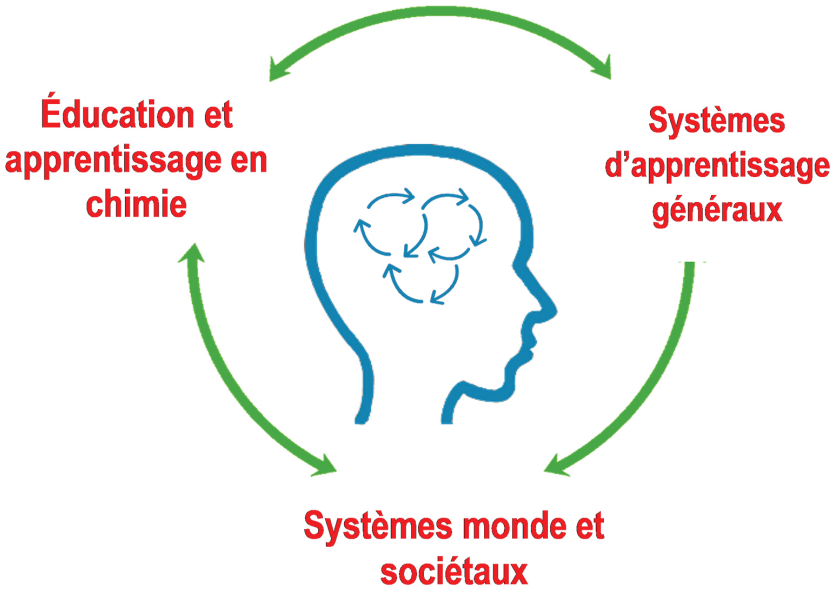

Figure 2. Framework for analysis of systems thinking in chemistry education

cross-disciplinary collaborations, or the active promotion of ethical behaviour, research integrity or equity, diversity and inclusion.

One major dilemma for chemistry organizations, including those representing chemistry at a national level and those focused on a particular sub-discipline or technique, is that many have become heavily dependent financially on the income they receive from publishing learned journals. Faced with the profound changes now taking place in the publishing world that are driven by the impact of rapidly evolving communications technologies (see also the section below on scientific publishing), there are threats to the sustainability of the organizations themselves as well as challenges to their representational and promotional roles on behalf of the discipline. The C4S group has advocated that the societies need to undertake a rebalancing of the priorities they give to publishing, compared with service to their membership and to the broader needs of the discipline and of society.

At the international level, chemistry organizations have often evolved as geographical or global federations of national chemical societies and industry associations, as well as of bodies that focus on a specific chemistry subject area, technique, process, or class of substance; or as new agents aiming to facilitate networking or the promotion of particular objectives. One especially important example is IUPAC, which was formally founded in 1919, includes many national chemical societies among its members and provides global networking opportunities through its diverse activities. Over time, a number of the international chemistry organizations have experienced stagnant or declining membership, stressed finances in an increasingly competitive environment, and outdated missions and archaic governance structures that no longer suit 21st century needs.

Considering how the diverse chemistry organization can adapt, in order to help lead and support the repositioning of the field as well as to ensure their own continued relevance and sustainability, led the C4S group to propose a menu of options for consideration. The menu includes a refreshing of the vision, mission, and organizational objectives and strategy; development of a clear, relevant international perspective; engagement in championing a refreshed chemistry education that is contemporary in its content, focus, and methodologies; a whole-hearted commitment to scientific publishing that is genuinely open access; development of models and strategies to restore and re-energise the academia/industry interface; a more active role in making the case to policy-makers, industry and the public for sustained, improved funding for the chemical sciences; submission to periodic, independent external evaluations to ensure good governance, fitness for purpose and effectiveness; and stronger engagement in actively promoting the value of the chemical sciences to diverse audiences in and beyond science.

7. Chemistry and health

Chemistry has made central contributions to improving health, wellbeing and life expectancy in the last two centuries, with both synthetic and analytical chemistry have played leading roles [25]. However, even greater contributions are needed now, when the world is experiencing a range of emerging and re-emerging infectious diseases, widespread resistance to antimicrobial agents, a growing global burden of non-communicable diseases and the impacts on health of a range of phenomena including planetary over-population, ageing societies, urbanization, environmental pollution and climate change.
Considering the interlocking systems of education, research, commercial development and regulation within which chemistry's contributions and impacts on health occur, the C4S group has identified a number of disconnections that are preventing the optimal contributions that the chemical sciences can make [26]. Interlinked systemic reforms are advocated, involving (1) re-contextualization of the chemistry/health interface through creating a recognized field of "the chemical sciences and health", which will strengthen teaching and research and prepare a body of chemical scientists trained in cross-

disciplinary working and able to undertake systems approaches to multi-faceted, complex problems; (2) determined and comprehensive efforts, by countries wishing to retain or strengthen their pharmaceutical development capacities, to reinforce their education, research, and innovation eco-systems; and (3) adoption of an integrated approach to the regulation of pharmaceuticals, food, and the environment.

8. Championing chemistry

The C4S group has highlighted the need for new champions of chemistry to step forward to help drive the reforms that are required in the discipline, ensure its continuing relevance to contemporary challenges and attract broad-based support and recognition of the contributions it makes to global progress [27].

It is argued that attracting the required champions must begin with developing a clarity of purpose and of commitment to ethical behaviour and solving societal challenges, such as that exemplified in the OWC framework. With this essential pre-requisite in place, the response to the question 'where are the champions' is that everyone must become champions: individual chemists, academic departments in colleges and universities, chemistry societies, environmental advocacy groups, government agencies, and industry. They must act both individually and collectively through coordinated initiatives. Within this overall shared responsibility, championing can be given leadership and afforded stronger public appeal and greater impact by encouraging the emergence of role models and skilled advocates.

9. Science in the 'post-truth' era

An especially important challenge, not only to chemistry but to the entire field of science and beyond, has emerged in what has come to be known as the 'post-truth' era [28]. Throughout history, there have been examples of the denial of facts and of evidence-based conclusions, but in recent decades this has emerged as a powerful phenomenon affecting opinions and behaviour on an unprecedented scale. The deliberate dissemination of lies, misinformation and untrue propaganda, including about facts and interpretations of science, has been seen in relation to issues such as vaccination to prevent serious and fatal diseases, health consequences of particular lifestyles, environmental pollution and climate change, as well as in connection with broader societal issues of economics and politics. The result has been the distortion of behaviours, policy positions, voting choices and lifestyle decisions, with impacts at individual, community, national and global levels.

The C4S group has drawn attention to the need for scientists generally, including chemists, to actively oppose this 'post-truth' tendency, combatting its insidious effects through actively denouncing lies, presenting true facts in a clear and comprehensible way to the public and policy makers, and espousing and advocating for the practice of 'scientific temper' [29-31]. This term was coined by Nehru [32] in 1946 to describe a way of life that rejects anti-science thinking. It is an individual and social process of thinking and acting, which uses the scientific method and which may, consequently, include questioning, observing physical reality, testing, hypothesizing, analysing and communicating. 'Scientific temper' describes an attitude which involves the application of logic. Discussion, argument and analysis are vital parts of scientific temper. Elements of fairness, equality and democracy are built into it.

Scientists and science institutions urgently need to establish and ensure the provision of resources for strategies that will help to educate and communicate to the public and policy-makers the significance and implications of advances and discoveries in science that impact on society and the environment. These communications should always emphasise the rigour of the scientific method and the dependence of science facts and theories on evidence that is tested and validated.

For the longer term, strengthening respect for valid science and wariness of post-truth tactics requires building a greater level of science literacy in society, the media and policy-makers.

Scientists themselves must act as models of good practice, operate a zero-tolerance policy towards all attempts to disseminate falsified and exaggerated data.

10. Scientific publishing

The C4S group has analysed the system of scientific publishing, with emphasis on a perspective from the chemical sciences [33]. They described a deep crisis that is unfolding, in which the present, flawed model for scientific publishing is damaging not only to science but also to the careers of many scientists and to the reputation of the field of scientific publishing as an honest, ethical and respected endeavour.

The analysis indicates that the crisis is being driven by the conjunction of sub-systems that connect the primary purpose of science publishing – that of scientific advancement to ensure that discoveries and theories are widely disseminated and exposed to critical examination – with financial and reputational rewards. These rewards, which create conflicts of interest for both authors and publishers, lead to severe distortions in behaviour, sometimes amounting to unethical or dishonest practices. Moreover, the increasing tendency to use bibliometric data as a surrogate for quality and scientific value has further distorted the reward and reputational systems.

The C4S group has argued that piecemeal solutions are unlikely to be effective or sustainable and the time is ripe for the stakeholders in science publishing to seek new, systemic approaches. These must comprehensively address the fundamental flaws in a ways that genuinely serve the interests of science, scholars and society. The reformed system must ensure equitable opportunity for all researchers – without regard to their prior scientific reputation, location or gender – to make their findings public, gain credit for the quality of their contributions and have open access to all the published work of others; and it must provide a high level of assurance to scientists, policy makers and the public about the reliability of the information accessed.

The outlines of an action plan for the science community to generate such a process are suggested. Key elements of this include simultaneously addressing the three intersecting elements of the scientific publishing system:

- Financial system: The central question that needs to be answered is: who pays, and how much, to achieve the most equitable and open access that is sustainable? Efforts must be made to go beyond the ‘gold’ and ‘green’ models, which enable open access for readers but still provide very large profits for publishers and encourage predatory practices and the creation of fake journals. Efforts must be made to reform the over-burdened peer-reviewing system and to minimise the costs of organizing and managing publishing, with an emphasis on paper-free, electronic formats in open repositories. Ultimately, the lowest costs will be generated if publishing is managed efficiently by not-for-profit entities. The more that publication costs and consequent fees charged to authors or users can be reduced, the lower will be the barriers to publication and access and the less will be the attractiveness to operators of predatory and fraudulent journals. There needs to be a serious debate, led by science academies and professional organizations and engaging scientists, policy makers, industry, science funders and foundations, about the best way to move open access forward sustainably. The European Union’s new open science initiative points to a promising avenue for development [34].
- Science advancement system: There is mounting evidence that the traditional peer reviewing system is no longer able to function effectively. There have been – and continue to be – massive increases in the number of papers being published, while the refereeing process itself is no longer reliable, since many examples are beginning to emerge where reviewers have failed to detect false data. There is also an increasing lack of confidence due to non-transparency and evidence of biases in the system and of randomness in outcomes. New models of review by peers are being explored and

are beginning to demonstrate the potential for reform, including review by groups of scientists on the web, in either fully open or semi-structured modes. These approaches can be ongoing, adding perspective to the correctness and value of the work over time. Further examination of these models and development of a universal approach is needed, through the joint effort of scientists, their institutions, archive centres and research funders. Whatever new system emerges, the integrity and fairness of decision-making needs to be robustly ensured through the rigorous application of scrutiny, adjudication and sanctions. Scientists who deliberately distort or falsify data must face penalties that are well defined, publicized and rigorously enforced, so that the public and policy-makers, as well as scientists, have confidence in system. This will require that science publishing is subjected to rigorous scrutiny that is independent of the scientists' institutions and the publishers.

- Reputational system: Current practices in the evaluation of scientific merit place excessive emphasis on metrics of publication numbers, the citation rates of papers and the status of the journals in which they appear. These metrics drive many of the worst features of the present scientific publishing system. In particular, they are used inappropriately for evaluating the extent of authors' contributions to the field and for judgements about career advancement, rather than employing qualitative judgements based on expert assessment. The San Francisco Declaration on Research Assessment (DORA) emphasizes that funders and institutions should acknowledge that *"the scientific content of a paper is much more important than publication metrics or the identity of the journal in which it was published"* and that publishers should *"greatly reduce emphasis on the journal impact factor as a promotional tool"* [35]. However, a more extensive initiative is now needed, which eradicates the use of all publication metrics for evaluations of authors' scientific contributions and the use of 'impact factors' as an indicator of journal quality. Academic institutions, funding agencies and bodies representing professional scientists should engage to generate a 'DORA 2' and to vigorously promote its universal application.

11. The chemical sciences and equality, diversity and inclusion

While the human right of all people to be treated fairly and without discrimination is enshrined in the UN's Universal Declaration [36], in practice many individuals and groups around the world suffer prejudice, exclusion and sometimes abuse and physical violence. The campaign to achieve equity, diversity and inclusion (EDI) in all areas has been gathering momentum around the world in recent years. The science community needs to be very actively engaged in this movement – not only to ensure that it is stamping out bad practices and ensuring EDI within its own institutions and practices, but also because progress in EDI will play an increasingly important role in advancing science itself, through the inputs made by the inclusion of individuals with more diverse backgrounds, experiences and perspectives, who will contribute to maximising innovation and creativity in science for the benefit of humanity [37,38]. It will enhance the capacity of science to tackle global problems and help achieve the SDGs and will help to create "a shared future in a fractured world [39].

In collaboration with Vivian Yam [40], the C4S group has discussed the challenge of dealing with conscious or unconscious forms of bias and discrimination in the sciences and argues that the chemical sciences can play a leading role in addressing biases, through (1) becoming a model of good systemic practice in policies, processes and actions; (2) developing practical skills through training in cultural competence; and (3) promoting a stronger evidence base, to uncover both the extent of problems and the degree to which approaches to improve equality, diversity and inclusion are working [41,42].

Conclusion

What began as a concern that chemistry urgently needed to undertake a repositioning to refresh both its internal dynamism and external image has become an evolving, detailed picture of the comprehensive nature of the reforms required.

Central themes that have emerged include the importance of a broader approach to education and practice in which greater emphasis is placed on cross-disciplinary approaches, systems thinking and the positioning of chemistry as a sustainability science and, overall, a science for the benefit of society. Applications of systems thinking to several facets of the science and societal milieus in which the chemical sciences operate have led to calls for specific and wide-ranging reforms in chemistry education, research and practice in general; as well as for major reforms in relation to areas such as chemistry and health, scientific publishing and the pursuit of equity, diversity and inclusion.
It is stressed that achievement of these reforms requires effort by all actors involved in the chemical sciences, including the educators, researchers, practitioners and professional bodies and associations at national and international levels. It will be necessary to tackle uncomfortable positions and vested interests to achieve the reforms. The prize will be the evolution of the next phase of this important science, generating increasing public confidence, support and understanding for its principles, processes, objectives and appreciation of its valuable capacities and products.

Biographical Sketches

Prof. Stephen Matlin is a former Professor in Biological Chemistry at the City University, London and Warwick University in the UK and a former Executive Director of the Global Forum for Health Research in Geneva. He is currently an Adjunct Professor in the Institute of Global Health Innovation at Imperial College London and Senior Fellow in the Global Health Centre at the Graduate Institute, Geneva. He is a member of the General Assembly and Head of Strategic Development at the International Organization for Chemical Sciences in Development.

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Prof Alain Krief is a French and Tunisian citizen. He is a former President of the Société Royale de Chimie (Belgium) and Director of the Laboratory of Organic Chemistry at the University Notre Dame de la Paix in Namur, Belgium and subsequently an Emeritus Professor there. He is a visiting Professor in the Hussain Ebrahim Jamal Research Institute of Chemistry, University of Karachi, Karachi,Pakistan. Since 2010 he has held the position of Executive Director of the International Organization for Chemical Sciences in Development.

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