บทความที่น่าสนใจประจำเดือนกันยายน 2559

สาขาวิทยาศาสตร์และเทคโนโลยี

1	Title:	Predicting skin permeation rate from nuclear magnetic resonance spectra
	Author:	Nan An, John-Hanson Machado, Yuechuan Tang, Jakub Kostal and Adelina Voutchkova-Kostal
	Journal:	Green Chemistry, Issue 16, 2016, pages 4468-4474
	Abstract:	In order to systematically approach the design of chemicals with minimal toxicity we are in need of predictive tools that can be applied seamlessly during chemical synthesis and characterization. Our approach is to develop models that utilize spectroscopic data, called Quantitative Spectrometric Data-Activity Relationships, to predict bioavailability and toxicity. Such models do not require knowledge of chemical structure and can be applied to chemical mixtures. Here we report a predictive QSDAR for skin permeation rate (log Kp) of organic chemicals from NMR spectroscopic data and molecular weight. The model is trained on a large data set consisting of structurally diverse chemicals and has been thoroughly externally validated – once with a withheld subset of the original data set, and once with a distinct set of complex biologically active compounds curated by Klimisch scoring (r2 = 0.838, qext12 = 0.837, qext22 = 0.419). The model performs equally or better than prevailing structure-based methods, and offers a number of advantages for facilitating rational design of safer chemicals.
	Database:	RSC

2	Title:	The ecotoxicogenomic assessment of soil toxicity associated with the production chain of 2,5-furandicarboxylic acid (FDCA), a candidate bio-based green chemical building block
	Author:	Guangquan Chen, Nico M. van Straalen and Dick Roelofs
	Journal:	Green Chemistry, Issue 16, 2016, pages 4420-4431
	Abstract:	2,5-Furan dicarboxylic acid (FDCA) is one of the top-12 value-added chemicals derived from biomass that may serve as a ‘green’ substitute for terephthalic acid (TPA) in polyesters. FDCA can be synthesized chemically from 5-(hydroxymethyl)furfural (HMF), which is produced from fructose or glucose. To investigate the impact of the production chain of FDCA on the terrestrial ecosystem and unravel molecular pathways affected in animals, an ecotoxicogenomic study was performed to measure the transcriptome-wide response in soil invertebrates, namely Folsomia candida. First, we show that FDCA, HMF and TPA are biodegradable in natural soil. However, these chemicals can exert severe impact on the reproduction of F. candida in sterilized soil. Transcriptional changes were examined at EC50 concentrations of FDCA, HMF and TPA spiked in sterilized LUFA 2.2 soils. The results indicate that FDCA and TPA cause no significant changes in gene expression, which may be due to the low chemical water solubility and therefore slow uptake from the pore water. In contrast, a substantial number of genes were significantly regulated in F. candida after exposure to HMF. Gene

	ontology analysis showed many biological processes to be significantly affected, such as nucleic acid metabolism, the transcriptional metabolic process, cell developmental process and oxidation–reduction process. Moreover, the transcriptional profiles suggest that HMF might be biotransformed by F. candida into 5-sulfoxymethylfurfural (SMF) which is genotoxic and mutagenic. Current research shows that the environmental risk of the FDCA production chain from biomass is relatively low, but may only be affected by the release of the intermediate HMF compound.
Database:	RSC

3	Title:	Aquatic ecotoxicity of personal care products: QSAR models and ranking for prioritization and safer alternatives' design
	Author:	Paola Gramatica, Stefano Cassani and Alessandro Sangion
	Journal:	Green Chemistry, Issue 16, 2016, pages 4393-4406
	Abstract:	Personal Care Product (PCP) ingredients, widely used all over the world, over the last few years have become chemicals of increasing environmental concern, mainly because they are detected in water and may harm wildlife. Due to their high structural heterogeneity, the big number of end-points and the huge lack of experimental data, it is very important to have tools able to quickly highlight the most hazardous and toxic compounds, focusing the experiments on the prioritized chemicals. In silico tools, like QSAR models based on structural molecular descriptors, can predict the missing data for activities and properties necessary to prioritize the existing or even not yet synthesized chemicals for their potential hazard. In the present study, new externally validated QSAR models, specific to predict acute PCPs' toxicity in three key organisms of aquatic trophic levels, i.e. algae, crustacean and fish, were developed according to the OECD principles for the validation of QSARs, using the QSARINS software. These OLS models based on theoretical molecular descriptors calculated by PaDEL-Descriptor software, selected by genetic algorithm, are statistically robust, externally predictive and characterized by a wide structural applicability domain. They were applied to predict acute toxicity for over 500 PCPs without experimental data; a trend of acute aquatic toxicity was highlighted by PCA allowing the ranking of inherently more toxic compounds, using also a MCDM approach for prioritization purposes. Additionally, a QSAR model for the prediction of this aquatic toxicity index (ATI) was proposed to be applicable in QSARINS for the a priori chemical design of non environmentally hazardous PCPs.
	Database:	RSC

4	Title:	Renewable and sustainable energy saving strategies for greenhouse systems: A comprehensive review
	Author:	Erdem Cuce, Dewanto Harjunowibowo, Pinar Mert Cuce
	Journal:	Renewable and Sustainable Energy Reviews, Volume 64, October 2016, Pages 34–59

Abstract:	In this study, a comprehensive review focusing on key strategies of energy saving and climate control technologies for greenhouses is presented. Following the brief and concise assessment of existing greenhouse systems in terms of their role in total energy consumption; cost-effective, energy-efficient and environmentally friendly technologies are analyzed in detail for potential utilization in greenhouses for notable reductions in energy consumption and emission levels. The technologies considered within the scope of this research are mainly renewable and sustainable based solutions such as photovoltaic (PV) modules, solar thermal (T) collectors, hybrid PV/T collectors and systems, phase change material (PCM) and underground based heat storage techniques, energy-efficient heat pumps, alternative facade materials for better thermal insulation and power generation (heat insulation solar glass, PV glazing, aerogel and vacuum insulation panel, polycarbonate sandwich panels), innovative ventilation technologies using pre-heating and cooling (high performance windcatchers) and efficient lighting systems. The findings from the research clearly reveal that up to 80% energy saving can be achieved through appropriate retrofit of conventional greenhouses with a payback period of 4–8 years depending on climatic conditions and crop type.
Database:	ScienceDirect

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Title:	A review on nanostructures of high-temperature thermoelectric materials for waste heat recovery
Author:	Fitriani, R. Ovik, B.D. Long, M.C. Barma, M. Riaz, M.F.M. Sabri, S.M. Said, R. Saidur
Journal:	Renewable and Sustainable Energy Reviews, Volume 64, October 2016, Pages 635–659
Abstract:	Alternative renewable energy sources are immensely important in view of the increase in worldwide energy needs and environmental effects. The thermoelectric (TE) technology is being seen as the perfect solution for both issues due to its ability to convert heat directly into electricity without CO2 emission. However, the application of TE materials for commercial devices is still limited due to their low conversion efficiency of ~10–15%. Currently the improvement of TE efficiency is challenging due to the relationship among physical properties, i.e., electrical conductivity, thermal conductivity and Seebeck coefficient which often counter each other and are restricted by the carrier concentrations. Fortunately, nanostructures have been shown to be able to disconnect the link among these physical properties to enhance the conversion efficiency of materials. Thus, the purpose of this review paper is to present the different nanostructured approaches for enhancing the TE properties of materials. The various techniques have been widely used to synthesize the bulk nanostructure and low dimensional systems were also described. A discussion on potential heat resources for the TE conversion, as well as the recent progress in TE is provided in terms of material, process and technology. Nanostructured skutterudites, half - Heusler, oxides and Si-Ge binary system were focused in this review paper due to the fact that the TE materials are among the best candidates for high-temperature applications. We also included our estimation in output electrical power of thermoelectric generation (TEG) for these

		type TE materials. Besides that, some innovations for the development of TE materials were mentioned. In addition, we also discussed the estimation of the TE cost to shed some light on commercializing considerations. We concluded that the high cost of the heat exchanger and ceramic substrate system components proved to be barriers in reducing the cost of TEG.
	Database:	ScienceDirect

6	Title:	Recent developments of control strategies for wind energy conversion system
	Author:	Ramji Tiwari, N. Ramesh Babu
	Journal:	Renewable and Sustainable Energy Reviews, Volume 66, December 2016, Pages 268–285
	Abstract:	Renewable energy technique is gaining more interest due to increasing demand and threat zero carbon foot prints. The energy from wind has a high potential as a source of energy. The growing demand of wind energy tends to produce a quality output power in terms of grid integration. An appropriate controller is required to control the power produce by the wind energy. A decent number of research publications reports had reviewed maximum power point tracking (MPPT), grid side controller (GSC) and machine side controller (MSC) associated with wind energy conversion system (WECS). However survey on pitch angle based control has not been focused exclusively in any such reviews. A concise review of pitch angle controller, maximum power extraction control and grid synchronisation controller is analysed in this paper. Thus, this paper presents a comprehensive review of overall control strategies for wind energy conversion control. The review paper is intended to provide a suitable reference for further research in the field of wind energy.
	Database:	ScienceDirect

7	Title:	Life Cycle Assessment of Power-to-Gas: Syngas vs Methane
	Author:	André Sternberg and André Bardow
	Journal:	ACS Sustainable Chemistry & Engineering, 2016, Volume 4, Issue 8, Pages 4156–4165
	Abstract:	Power-to-Gas enables the integration of renewable electricity and carbon into the chemical industry. The electricity is used to produce hydrogen, which is subsequently converted with CO2 as the renewable carbon source. The resulting products can be used as feedstock for the chemical industry replacing current fossil-based feedstock. Because the integration of renewable electricity and carbon into the chemical industry is mainly environmentally motivated, we identify the conditions under which Power-to-Gas pathways are environmentally beneficial. The conditions are expressed as environmental threshold values for electricity supply. The threshold values are derived by a comparative life cycle assessment (LCA) of Power-to-Gas pathways to fossil-based processes. We analyze Power-to-Gas pathways to synthetic natural gas (Power-to-SNG) and to syngas (Power-to-Syngas). SNG is produced by the Sabatier reaction; syngas by reverse water gas shift (rWGS) and dry reforming of methane

		(DRM). The threshold values for electricity supply allow us to compare the environmental benefit of Power-to-SNG and Power-to-Syngas on an equal basis: how well they utilize the currently limited renewable electricity. Syngas production by the DRM process has the largest environmental potential. Both Power-to-Syngas pathways lead to larger environmental benefits than Power-to-SNG making syngas the more desirable product than methane as long as renewable electricity is limited.
	Database:	American Chemical Society Journal (ACS)

8	Title:	Highly Flexible Strain Sensor from Tissue Paper for Wearable Electronics
	Author:	Yuanqing Li, Yarjan Abdul Samad, Tarek Taha, Guowei Cai, Shao-Yun Fu, and Kin Liao
	Journal:	ACS Sustainable Chemistry & Engineering, 2016, Volume 4, Issue 8, Pages 4288–4295
	Abstract:	We introduce a simple method to fabricate a highly flexible resistive-type strain sensor composed of carbon paper (CP) and polydimethylsiloxane (PDMS) elastomer. The key resistance sensitive material of the sensor, carbon paper, is prepared from tissue paper by a simple high-temperature pyrolysis process. At the same time, the as-fabricated CP/PDMS strain senor is highly sensitive to applied strain with a gauge factor of 25.3, almost 10 times higher than that of conventional metallic strain gauge. Furthermore, the response of CP/PDMS strain sensor under cyclic tensile strain with a peak strain of 3% was also investigated, which exhibits fast and steady response with excellent durability within the frequency range 0.01–10 Hz. Finally, we demonstrate the successful utilization of the CP/PDMS strain sensor as wearable electronics in breath monitoring and robot controlling. The eminent performance, low material cost, and facile fabrication process make the CP/PDMS strain sensor exceptionally promising in flexible, stretchable, and wearable electronics.
	Database:	American Chemical Society Journal (ACS)

9	Title:	Ex-ante sustainability assessment of cleaner banana production systems
	Author:	Pierre Chopin, Jérôme Tirolien, Jean-Marc Blazy
	Journal:	Journal of Cleaner Production, Volume 139, 15 December 2016, Pages 15–24
	Abstract:	As one of the largest users of pesticides in the world, banana production is responsible for numerous types of pollution affecting water, soil and air and causing a variety of health issues. Agroecological innovations can help to reduce pesticide use and achieve cleaner and more sustainable banana production systems. Innovations must be well suited to the diversity of banana farms and acceptable to the stakeholders involved in production. We tested the impact of 18 agroecological innovations in Guadeloupe on the sustainability of three contrasted production systems, using the multi-criteria assessment model MASC. These innovations included different types of fallow (A), bans on pesticides (B), conditional applications of pesticides (C), intercropping (D), resistant cultivars (E), and integrated systems (F). In the assessment, we introduced the views of 29 stakeholders involved in sustainability

	issues relative to banana grouped through three sets of weightings, obtained by direct weighting of the indicators used in a multi-criteria assessment tool. We analysed the effects of each set of weightings on the sustainability level for these different banana production systems. Our results showed that the adoption of innovations can have negative, positive or no effects on the overall sustainability of banana production systems. Although none of the innovations had a positive effect on all cropping systems, some innovations were relevant to several farm types. However, this depended on the sets of weightings considered, because we found several types of stakeholder with opposing views on the importance of sustainability components. Integrated and organic systems produced the best results in terms of increasing sustainability and were relevant to current farming systems. However, in order to obtain cleaner banana production at the landscape scale, a combination of these innovations, tailored to the diversity of farmers' situations and stakeholder preferences, still needs to be proposed.
Database:	ScienceDirect

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Title:	Daily forecast of solar thermal energy production for heat storage management
Author:	Sylvain Rodat, Christian Tantolin, Xavier Le Pivert, Sylvain Lespinats
Journal:	Journal of Cleaner Production, Volume 139, 15 December 2016, Pages 86–98
Abstract:	Solar energy offers a renewable source of power but its fluctuating nature raises concerns about the electrical grid balancing. Network regulators have to estimate the upcoming production to match supply with demand; consequently, power plant operators may be asked to provide accurate forecasts. Planning the thermal or electrical output of solar power plants is thus highly required to ensure a stable power chain supply. This paper presents a solution that couples a meteorological model with a solar power plant performance model. The power output is predicted 24 h ahead in the case of a solar Fresnel power plant. The required Direct Normal Irradiance is inferred from the global horizontal irradiance; the thermal production is evaluated from an optical and thermal model. Our approach has been validated on a 1000 m2 Fresnel power plant, paving the way for model-based storage strategy.
Database:	ScienceDirect