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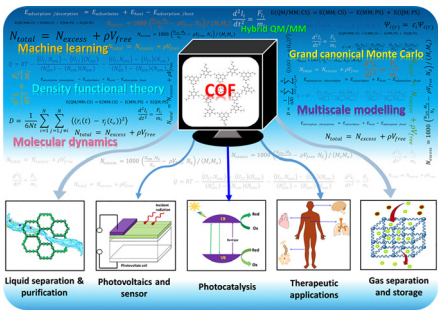
**Exploring covalent organic frameworks through the lens of computational chemistry**

Parashmoni Rajguru, Prarthana Bora, Chinmoy Bhuyan and Swapnali Hazarika*

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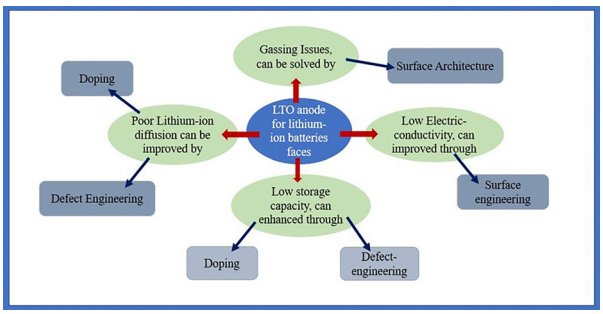
**The role of atomic-level understanding in optimizing lithium titanate oxide based anodes for lithium-ion batteries**

Emaan Shahid and Abdul Majid*



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## REVIEWS

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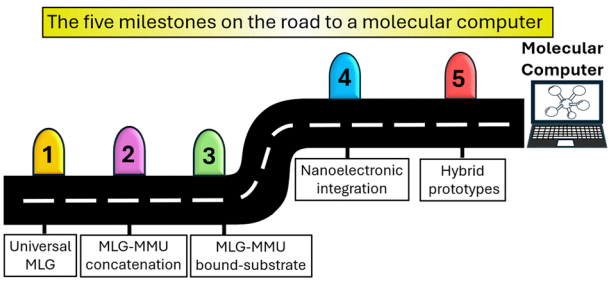
**Assembling a molecular computer: challenges in integrating molecular logic, memory, and interconnects from the "bottom-up"**

Alexander Ciupa*

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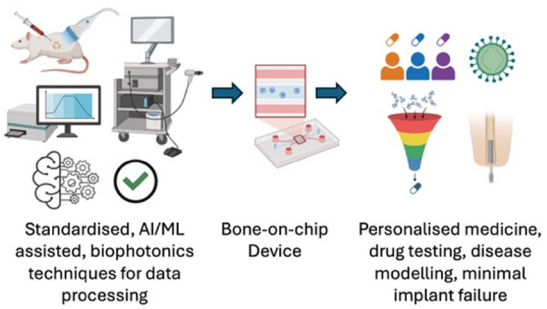
**Integration of biophotonics with bone-on-chip technology for continuous, non-invasive monitoring of bone regeneration**

Imanda Jayawardena,* Stefan Andersson-Engels and Rekha Gautam

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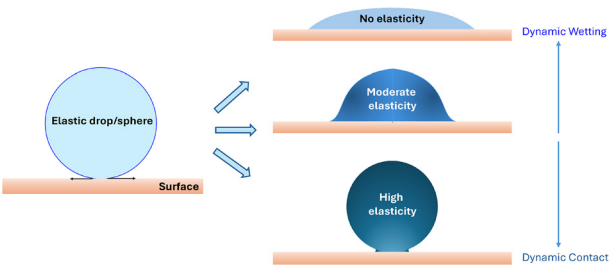
**Short-time spreading dynamics of elastic drops**

Surjyasish Mitra, A-Reum Kim, Boxin Zhao and Sushanta K. Mitra*

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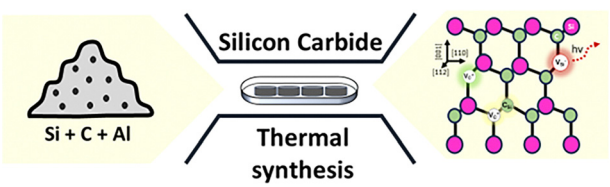

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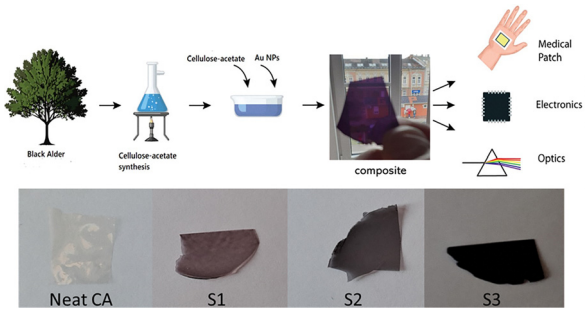


**Gold nanoparticle-embedded cellulose acetate: structural, optical, mechanical, and cytotoxicity assessment**

Mislav Mustapić,* Maja Molnar, Nikola Španić, Mario Komar, Barbara Viljetić, Ljubica Glavaš-Obrovac, Marija Heffer, Boštjan Genorio, Ana Ivković, Rafael Anelić, Fabio Faraguna, Lázár Tóth, Judit Budai, Zsuzsanna Márton and Domagoj Belić*

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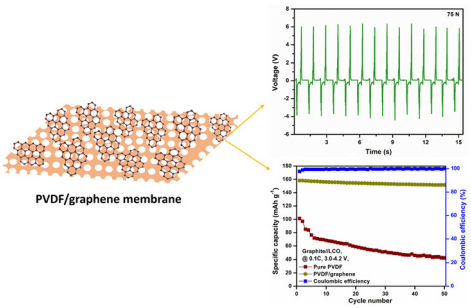


**Graphene-PVDF composite membrane for piezoelectric nanogenerators and lithium-ion batteries**

Ashok Kushwaha,* Anu Teresa Peter, Faiz Ullah Shah* and Dipti Gupta*

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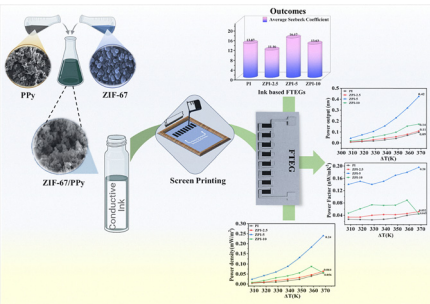


**A decoupling strategy to optimize power density in flexible thermoelectric devices using a ZIF-67 doped polypyrrole bio binder-based hybrid ink**

Kishor D. Kalarakoppa, A. N. Prabhu,* Ramakrishna Nayak, Nishitha Prabhu, Mohammad Saquib, Shilpa Shetty and Kavya Naik

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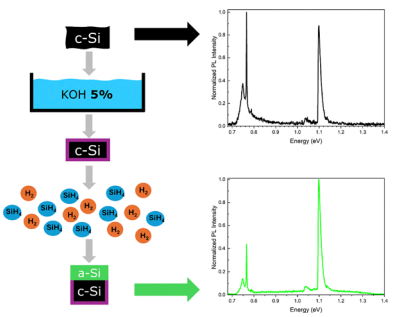


**Optimization of the crystalline silicon surface by chemical treatment and hydrogenated amorphous silicon: a photoluminescence study**

Maria B. Candeias,* Ghulam Abbas, Alexandr Zamchiy, Rodrigo Martins, Manuel J. Mendes, Hugo Águas, Rui N. Pereira and Joaquim P. Leitão*



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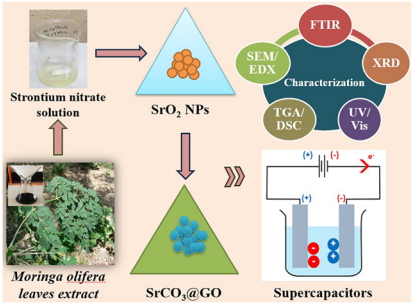
***Moringa oleifera*** **mediated synthesis of $SrO_2$ and $SrCO_3$@GO nanomaterials for energy storage applications**

Rabia Kashif, Shabbir Hussain,* Israr Ahmad, Muhammad Tariq, Muhammad Imran, Muhammad Ibrar, Farhana Bibi, Khurram Shahzad Munawar, Muhammad Waqas and Sami Ullah

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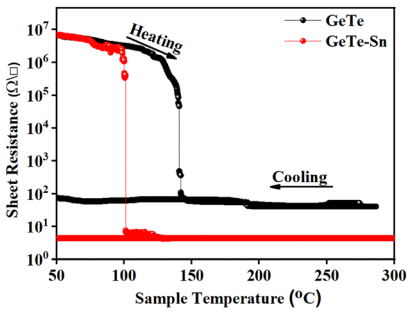
**Controlling the phase transition dynamics of GeTe by Sn substitution for phase change memory, photodetection and neuromorphic devices**

Mubaris N. K., Rajkumar Shanajaoba Singh, Prabhukrupa Chinmay Kumar, Ramakanta Naik and Vinod E. Madhavan*

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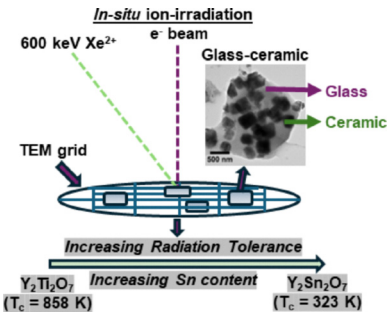


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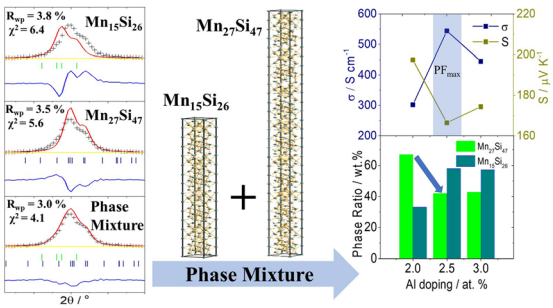
**Structural and thermoelectric properties of $Mn(Si_{1-x}Al_x)_{1.75}$: a commensurate phase mixture approximation**

Panagiotis Mangelis,* Panagiotis S. Ioannou, Anne-Karin Søiland and Theodora Kyratsi



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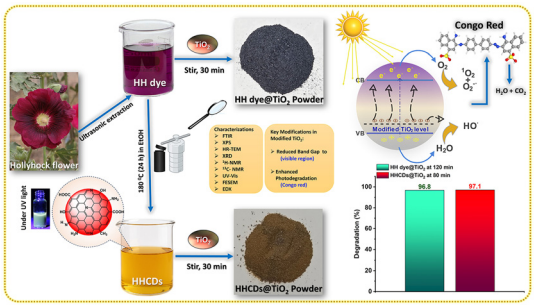


**Sustainable $TiO_2$ photocatalysts modified with hollyhock-derived carbon dots and natural dye for enhanced visible-light degradation of Congo red: a comparative study**

Govar H. Hamasalih, Sewara J. Mohammed* and Shujahadeen B. Aziz*

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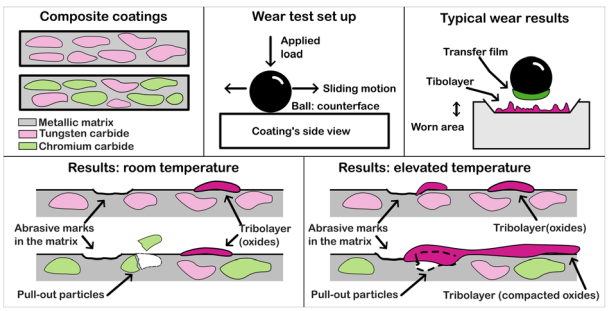


**Effect of carbide on wear mechanisms at 300 °C of composite coatings sprayed by HVOF**

Alejandra Islas Encalada,* Pantcho Stoyanov, Mary Makowiec, Christian Moreau and Richard R. Chromik*

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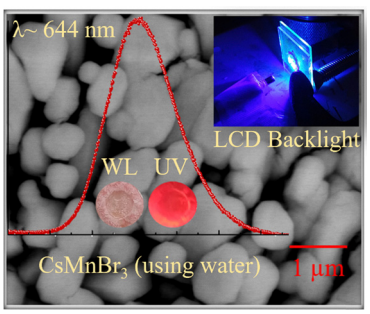


**Low temperature green synthesis of red emitting Pb-free $CsMnBr_3$ perovskite films**

Saurabh Singh,* Xiyu Wen and Fuqian Yang

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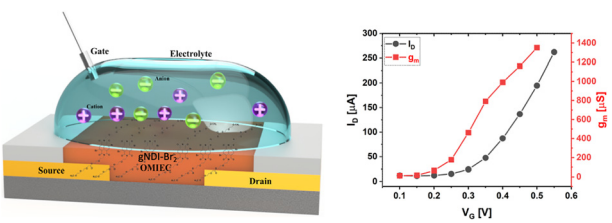


**Optimization of drop-casting parameters for fabrication of n-type accumulation mode organic electrochemical transistors (OECTs) using gNDI-$Br_2$**

Seongdae Kang, Jiaxin Fan and Manisha Gupta*



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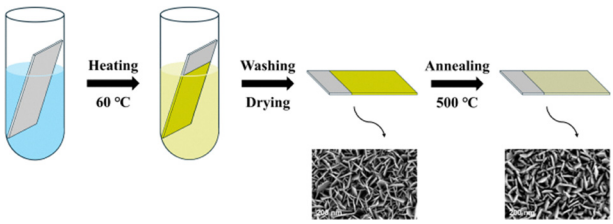
**Optimizing transmittance in $WO_3$-based electrochromic films: advanced growth control *via* chemical bath deposition**

Jiacheng Yao,* Gai Lin and Min Zhang*

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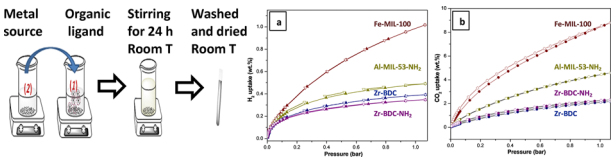
**Selected sustainably synthesized metal–organic frameworks for hydrogen and carbon dioxide storage**

Nejat Redwan Habib, Isabel Diaz, Abi M. Taddesse and Henrietta W. Langmi*

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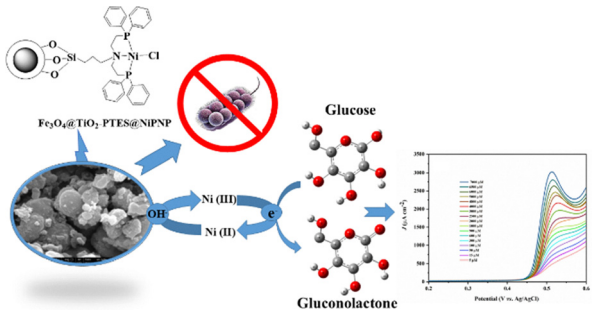
**Synthesis of a hybrid material based on a high-surface-area magnetic $Fe_3O_4$@$TiO_2$ core–shell structure and immobilized Ni–PNP aliphatic pincer complex: study of the structural, magnetic, and antibacterial properties and nonenzymatic electrochemical sensing of glucose**

Fatemeh Ariaeinezhad, Gholamhossein Mohammadnezhad,* Oluseun Akintola and Winfried Plass*

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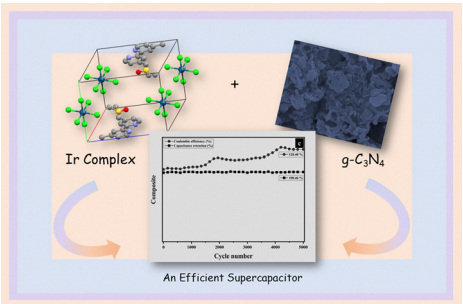
**Synthesis and characterization of a nanocomposite of an iridium-based complex with mesoporous g-$C_3N_4$ and its application as a supercapacitor**

Mohammad Yaghoubi, Vahid Amani,* Faranak Manteghi* and Edris Jamshidi



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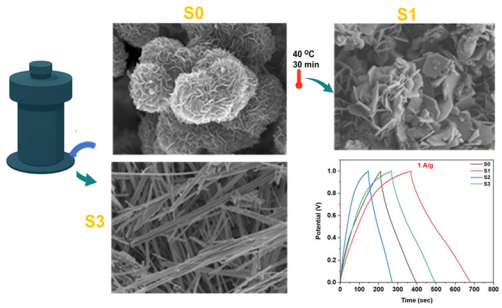


**Morphology-engineered α-$MoO_3$ nanostructures *via* $MoS_2$ transformation for high-performance supercapacitors**

Ahmed A.R. Abdel-Aty, Mohammed Mosaad Awad, Olfa Kanoun and Ahmed S.G. Khalil*

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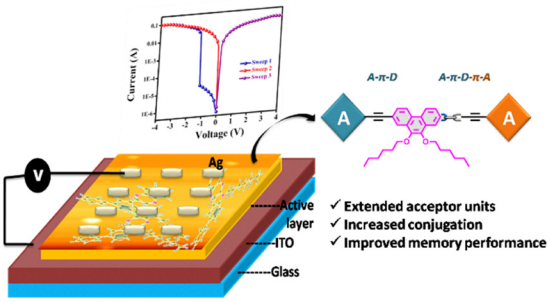


**Exploring the influence of acceptor-strength in alkoxyphenanthrene-based A–π–D–π–A *versus* D–π–A architectures for resistive WORM memory devices**

Senthilkumar V. Swetha, Murali Ardra, Predhanekar Mohamed Imran and Samuthira Nagarajan*

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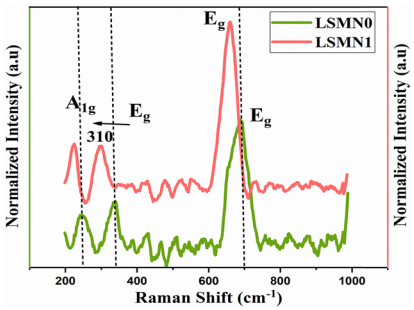


**Tailoring structural and optical responses in rhombohedral $La_{0.67}Sr_{0.33-x}Ca_xMn_{1-x}Ni_xO_3$ through dual-site doping**

Zouhayra Aydi,* Radhia Dhahri, Essebti Dhahri, El-Kébir Hlil and E. López-Lago

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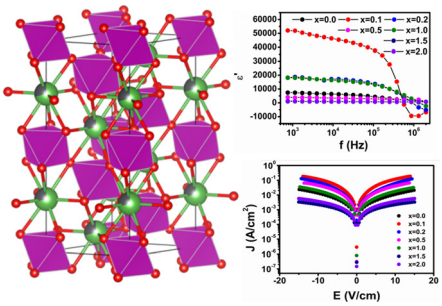


**Re-entrant structural phase transition and charge carrier conduction in $La_{2-x}Sr_xFeMnO_6$ solid solutions for electronic device applications**

Baniya R. Meena and Anup K. Ghosh*



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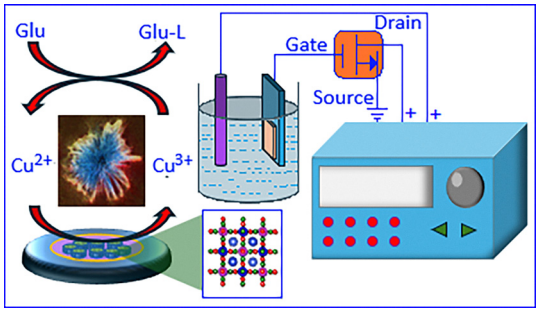
**Complexation-driven synthesis of potassium copper ferrocyanide nanoparticles for nonenzymatic glucose detection: an electrochemical and FET-based approach**

Chandan Saha, Pooja Kumari, Mustafizur Hazarika and Kaushik Mallick*

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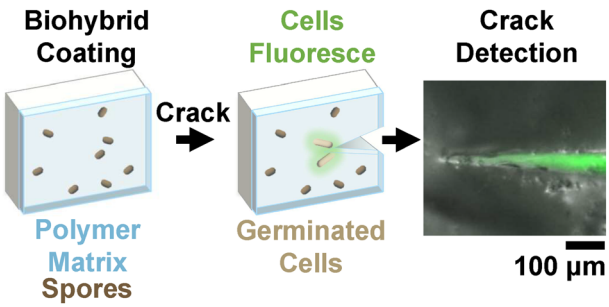
**Mechanically driven bacteria-based crack detection**

Ellen W. van Wijngaarden, Tyrone Chen, Ilana L. Brito, Nikolaos Bouklas, Andrea Giometto and Meredith N. Silberstein*

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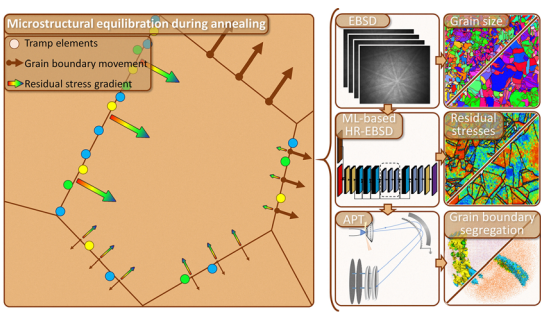
**Tramp element drag on grain boundaries controlling microstructural and residual stress equilibration in copper thin-films**

Charlotte Cui, Rahulkumar Sinojiya, Bernhard Sartory, Michael Tkadletz, Michael Reisinger, Johannes Zechner, Werner Robl and Roland Brunner*

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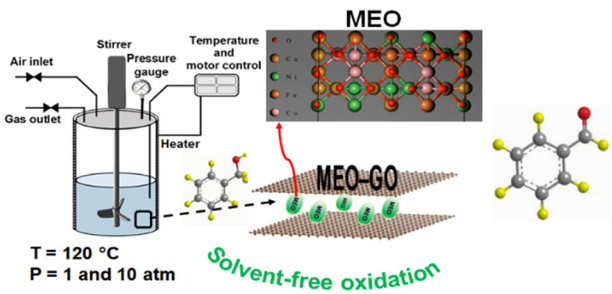
**A comparative study of medium-entropy oxide and metal oxide nanoparticles on graphene oxide for benzyl alcohol oxidation under solvent-free conditions**

Seyedsaeed Mehrabi-Kalajahi,* Seyed Amir Hossein Vasigh, Behrouz Shaabani,* Hassan Yousefi Bavili, Ahmad Ostovari Moghaddam, Ameen Al-Muntaser and Mikhail A. Varfolomeev



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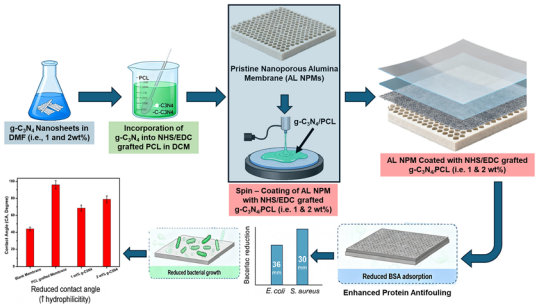


**Innovative polycaprolactone/graphitic carbon nitride composite coatings: enhancing the antibacterial properties of nanoporous alumina membranes**

Ahmed N. Emam,* Lamyaa Osama, Hanan H. Beherei and Mostafa Mabrouk*

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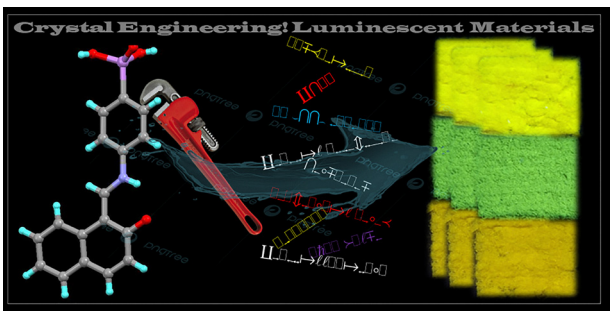


**Optical studies of stimuli-responsive organic crystals differing in the position and nature of functional groups**

Sumeera Farooq, Ishtiyaq Ahmad and Aijaz A. Dar*

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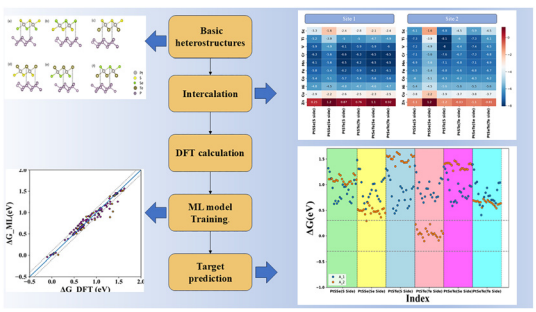


**Machine learning screening and high-throughput computation of 3d-transition-metal intercalated Janus PtXY/ζ-phosphorene (X ≠ Y; X, Y = S, Se, Te) heterostructures for photocatalytic water splitting**

Sreesanth Kolangaravalappil, Ramandeep Singh, Pooja Jamdagni and Ashok Kumar*

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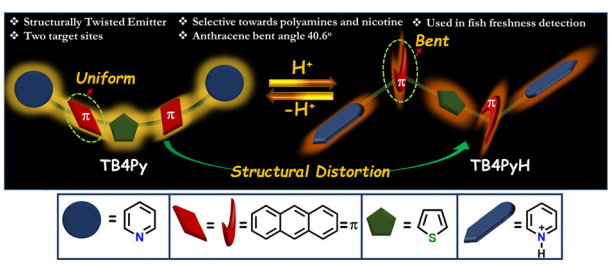


**Protonation-driven structural deformation in a conformationally twisted pyridyl-linked AIEgen: a platform to detect polyamines and nicotine**

Madhuparna Chakraborty, Avanigadda Madhu Niharika, Zubair Khalid Baig and Manab Chakravarty*



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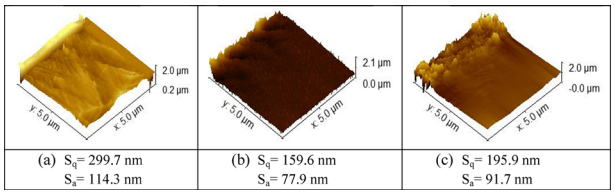
1188

**Bio-based surface treatments for concrete durability: exploring the corrosion-inhibiting properties of *Costus afer* and *Chrysophyllum albidum* leaf extracts on fungal growth**

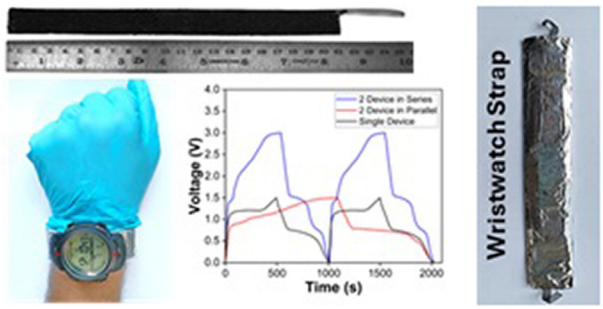
Uzoma Charles Chukwuma,* Joan Ijeoma Arimanwa, Kanayo Lucy Oguzie, Ugochi Nneka Kemka, Ini-Ibehe Nabuk Etim, Sikandar Khan, Kingsley O. Ukaegbu and Emeka Emmanuel Oguzie




1203

**Ni–Cu–Mn based hybrid supercapacitor with high flexibility and strength for wearable electronics**

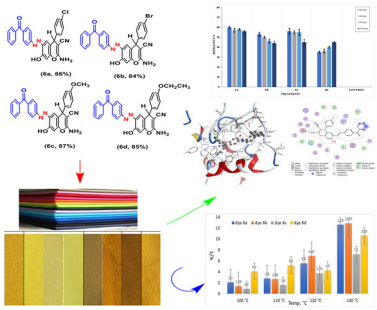
Arunesh Kumar, Arpit Thomas, Michael Lastovich, Bharat Gwalani and Harpreet Singh Arora*




1213

**Innovative chromene-based disperse dyes for concurrent dyeing: molecular docking, biochemical assessment, and repellent efficacy against *Culex pipiens* mosquitoes**

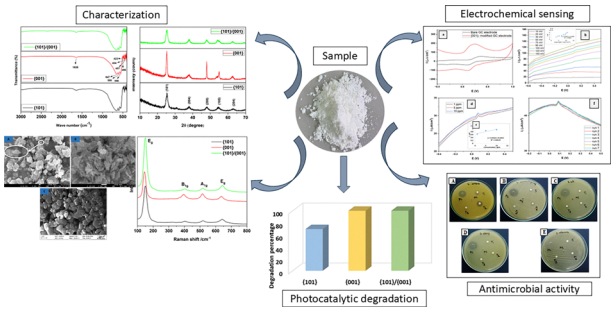
Mohamed S. A. El-Gaby, M. A. Habib, Nadeem Raza, Ahmed B. M. Ibrahim, Ali A. Ali,* Walid E. Elgammal, Ahmed H. Halawa, Mostafa A. Ismail, Tharwat A. Selim, Ahmed I. Hasaballah, Mohamed A. M. El-Tabakh and Gameel A. M. Elhagali



1233

**Exploring facet-engineered anatase nanoparticles for amplification of sensitivity in heavy metal ion detection and other applications**

Md. Anayet Ullah, Fataha Nur Robel, Newaz Mohammed Bahadur, Dipa Islam, Subarna Sandhani dey, Samina Ahmed* and Md. Sahadat Hossain*



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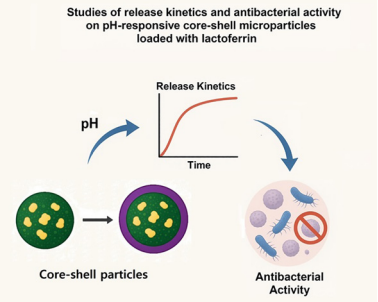
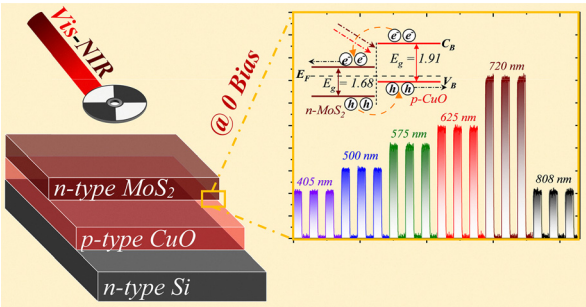
1250




**Studies of release kinetics and antibacterial activity on pH-responsive core–shell microparticles loaded with lactoferrin**

Teresa Paduano, Michela Salamone, Federica Carraturo, Simona Zuppolini,* Mauro Zarrelli, Aldobenedetto Zotti, Rosa Vitiello, Marika Avitabile, C. Valeria L. Giosafatto, Marco Guida, Riccardo Tesser and Anna Borriello

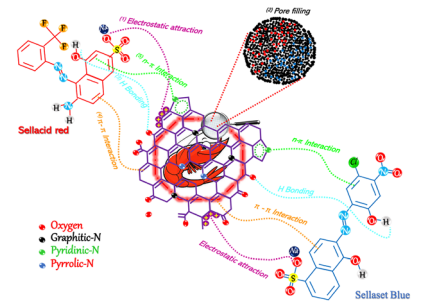
1265




**Self-biased visible-NIR photodetection enabled *via* a dual-heterojunction n-$MoS_2$/p-CuO/n-Si design**

Tabark A. Fayad, Mohamed Hassan Eisa, Ethar Yahya Salih* and Asmiet Ramizy

1272




**Shrimp shell-derived chito-protein nanocomposites for sustainable dye effluent remediation: efficiency, reusability, and environmental safety**

Nisrine Nouj,* Zineb Majbar, Ingrid Ioana Buciscanu, Aboubakr Ben Hamou, Ayoub Chaoui, Mohamed Rida Abelouah, Mohamed Idbella, Abdelaziz Ait Addi, Nadia Eladlani, Ali Zourif, Mohamed Benafqir, Naima Hafid, Igor Cretescu, Amane Jada and Noureddine El Alem

1291

**Flexible donor–acceptor nanocomposite for triggered photocatalytic $CO_2$ fixation *via* an artificial leaf approach**

Kuldeep Kumar, Rajesh K. Yadav,* Rajesh K. Verma,* Sanjay Mishra, Kanchan Sharma, Rehana Shahin, Shaifali Mishra, Satyam Singh, Atul P. Singh, Navneet K. Gupta and Jin OoK Baeg*



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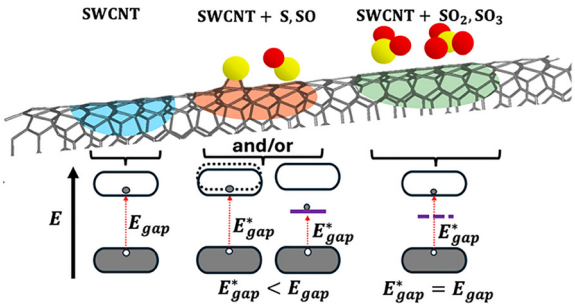
## PAPERS

1303

**First-principles investigation of sulfur and sulfur-oxide compounds as potential optically active defects on (6,5) SWCNT**

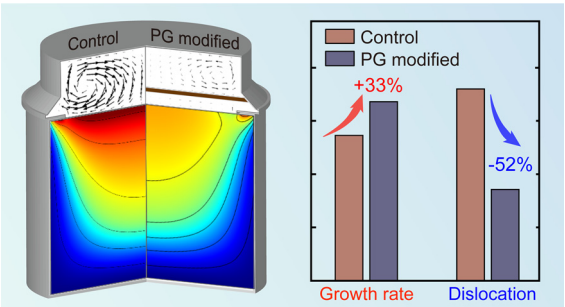
Tina N. Mihm,* Kasidet Jing Trerayapiwat, Xinxin Li, Xuedan Ma and Sahar Sharifzadeh




1311

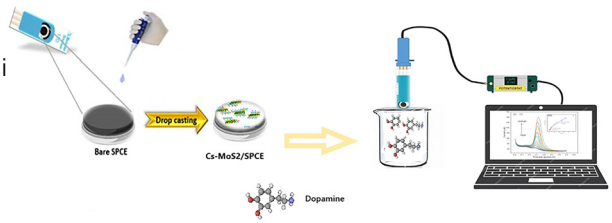
**Porous graphite plate design in SiC PVT growth: optimized powder source evolution for enhanced crystal yield and quality**

Yang Chen, Xiaofang Ye, Shilin Liu, Wenyu Kang,* Wei Jiang, Jun Yin* and Junyong Kang




## CORRECTION

1321

**Correction: Advanced 2D $MoS_2$–chitosan nanocomposites for ultra-sensitive and selective dopamine detection**

Ratiba Wali, Rayhane Zribi,* Viviana Bressi, Ramzi Maalej, Antoni Wissem Cheikhrouhou-Koubaa and Giovanni Neri