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REVIEWS

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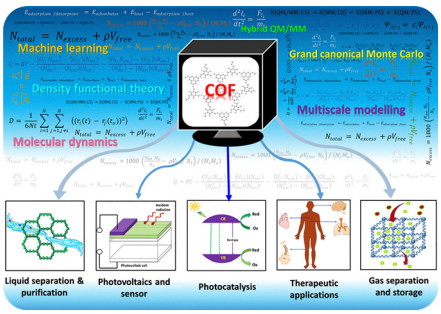
Exploring covalent organic frameworks through the lens of computational chemistry

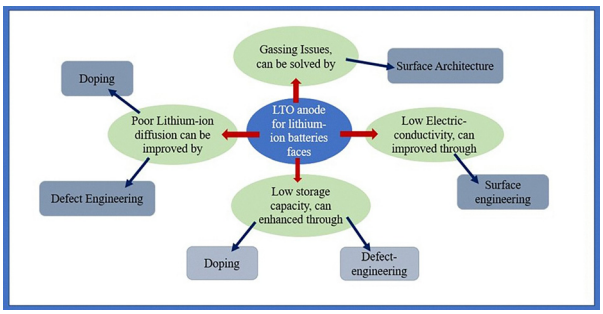
Parashmoni Rajguru, Prarthana Bora, Chinmoy Bhuyan and Swapnali Hazarika*



715

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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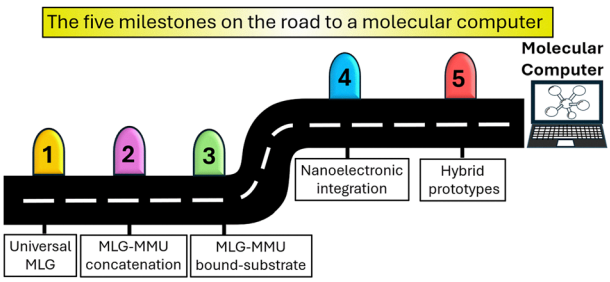
REVIEWS

733

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

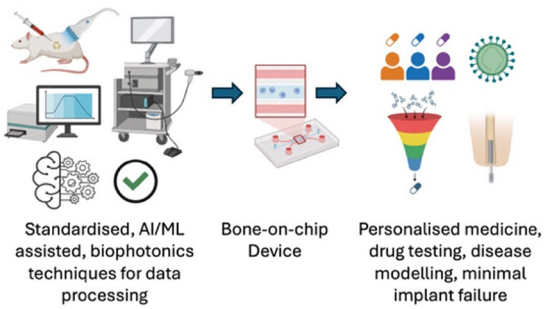
Alexander Ciupa*



750

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

Imanda Jayawardena,* Stefan Andersson-Engels and Rekha Gautam

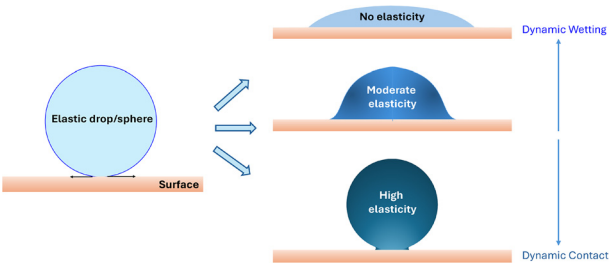


PAPERS

772

Short-time spreading dynamics of elastic drops

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



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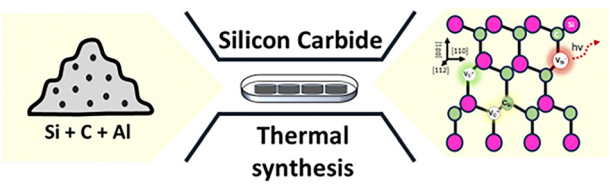
The role of aluminum in controlling defect formation and polytypism in silicon carbide *via* thermal synthesis

Sarah Morais Bezerra, Sándor Kollarics, Luisa Souza Almeida, Gábor Bortel, Nikoletta Jegenyés, Bence Gábor Márkus, Ferenc Simon, Adam Gali* and David Beke*



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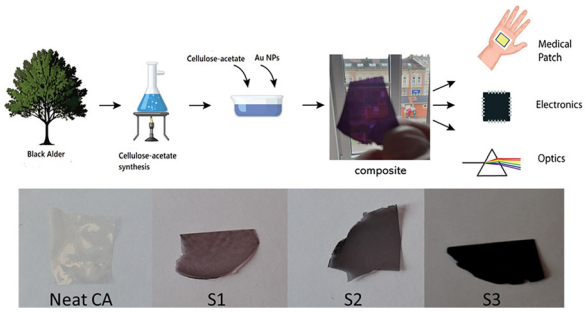

Gold nanoparticle-embedded cellulose acetate: structural, optical, mechanical, and cytotoxicity assessment

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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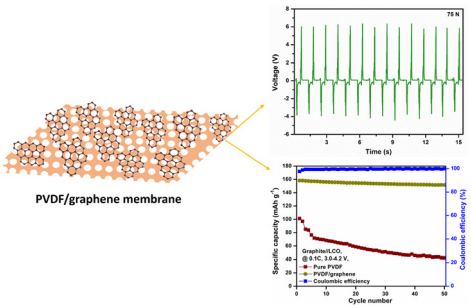

Graphene-PVDF composite membrane for piezoelectric nanogenerators and lithium-ion batteries

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

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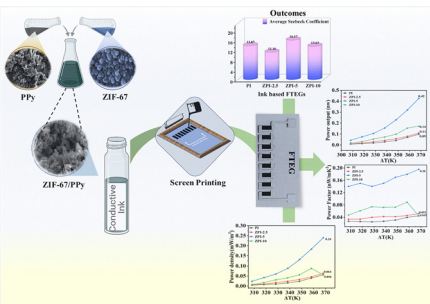

A decoupling strategy to optimize power density in flexible thermoelectric devices using a ZIF-67 doped polypyrrole bio binder-based hybrid ink

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

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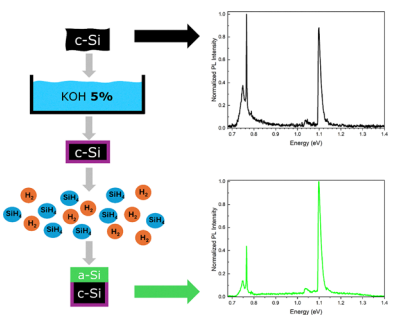

Optimization of the crystalline silicon surface by chemical treatment and hydrogenated amorphous silicon: a photoluminescence study

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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PAPERS

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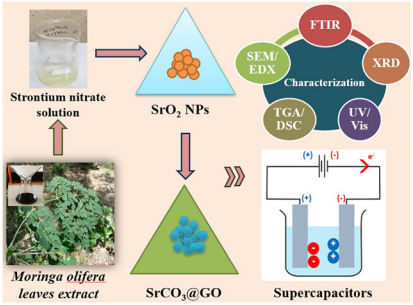
Moringa oleifera **mediated synthesis of SrO_2 and $SrCO_3$@GO nanomaterials for energy storage applications**

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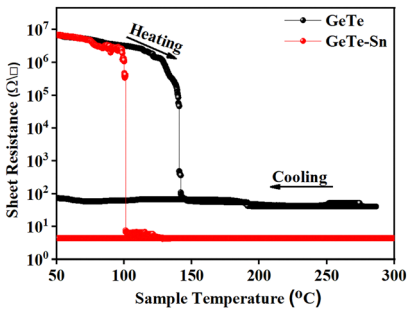
Controlling the phase transition dynamics of GeTe by Sn substitution for phase change memory, photodetection and neuromorphic devices

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



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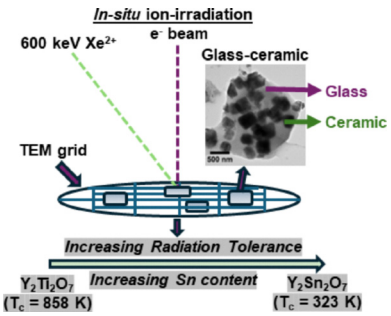
Tuning the radiation tolerance of titanate pyrochlore *via* Sn-substitution: an *in situ* ion irradiation study of pyrochlore-glass ceramics

Mohamed Ruwaid Rafiuddin,* Anamul Haq Mir,* Linggen Kong and Yingjie Zhang



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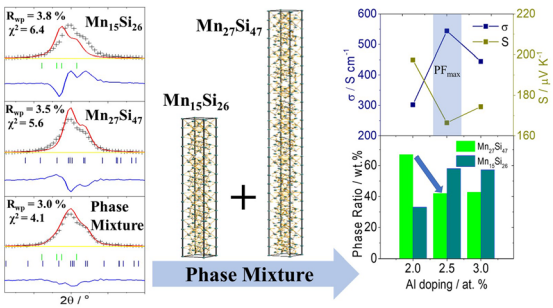
Structural and thermoelectric properties of $Mn(Si_{1-x}Al_x)_{1.75}$: a commensurate phase mixture approximation

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



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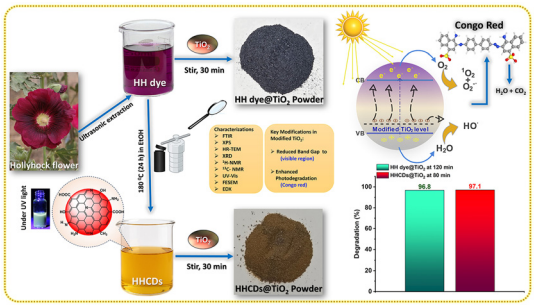

Sustainable TiO_2 photocatalysts modified with hollyhock-derived carbon dots and natural dye for enhanced visible-light degradation of Congo red: a comparative study

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

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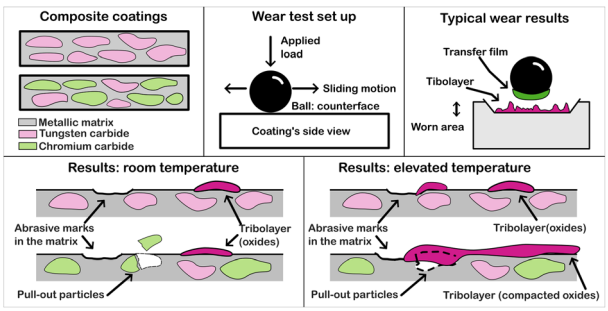

Effect of carbide on wear mechanisms at 300 °C of composite coatings sprayed by HVOF

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

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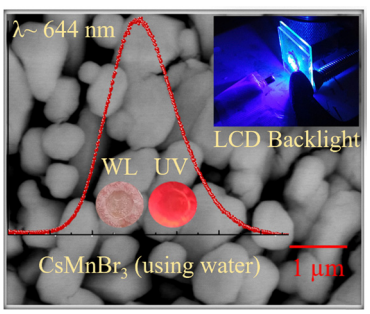

Low temperature green synthesis of red emitting Pb-free $CsMnBr_3$ perovskite films

Saurabh Singh,* Xiyu Wen and Fuqian Yang

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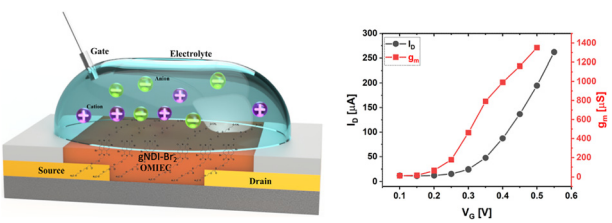

Optimization of drop-casting parameters for fabrication of n-type accumulation mode organic electrochemical transistors (OECTs) using gNDI-Br_2

Seongdae Kang, Jiaxin Fan and Manisha Gupta*

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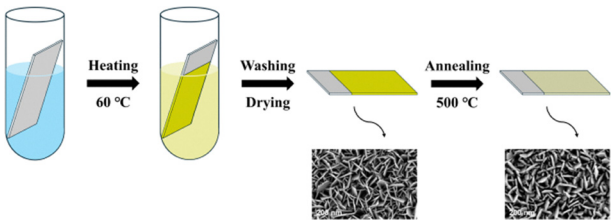
Optimizing transmittance in WO_3-based electrochromic films: advanced growth control *via* chemical bath deposition

Jiacheng Yao,* Gai Lin and Min Zhang*



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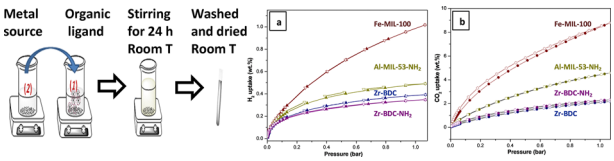
Selected sustainably synthesized metal–organic frameworks for hydrogen and carbon dioxide storage

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



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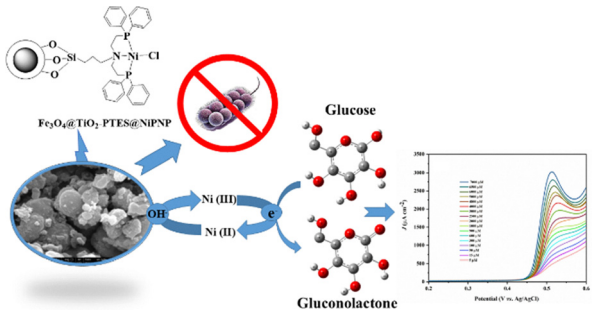
Synthesis of a hybrid material based on a high-surface-area magnetic Fe_3O_4@TiO_2 core–shell structure and immobilized Ni–PNP aliphatic pincer complex: study of the structural, magnetic, and antibacterial properties and nonenzymatic electrochemical sensing of glucose

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



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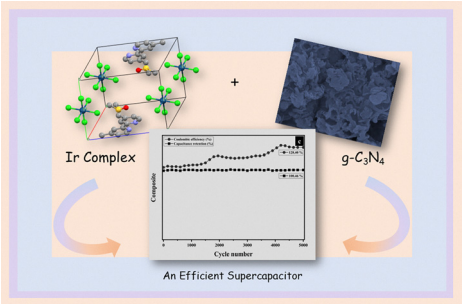
Synthesis and characterization of a nanocomposite of an iridium-based complex with mesoporous g-C_3N_4 and its application as a supercapacitor

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



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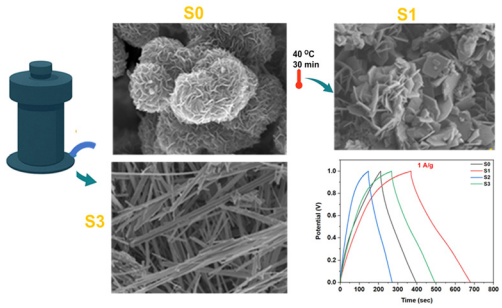

Morphology-engineered α-MoO_3 nanostructures *via* MoS_2 transformation for high-performance supercapacitors

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

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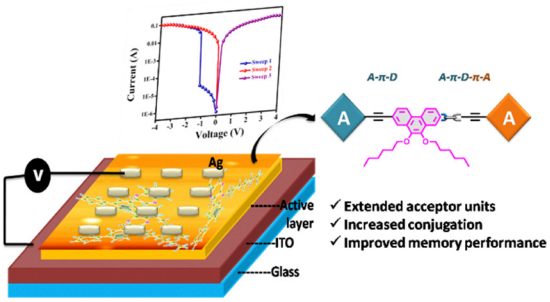

Exploring the influence of acceptor-strength in alkoxyphenanthrene-based A–π–D–π–A *versus* D–π–A architectures for resistive WORM memory devices

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

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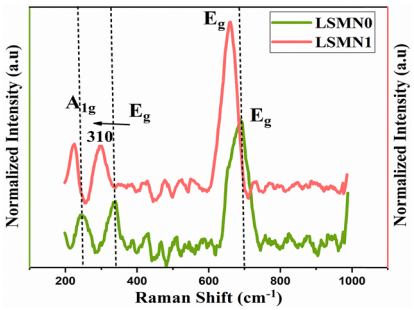

Tailoring structural and optical responses in rhombohedral $La_{0.67}Sr_{0.33-x}Ca_xMn_{1-x}Ni_xO_3$ through dual-site doping

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

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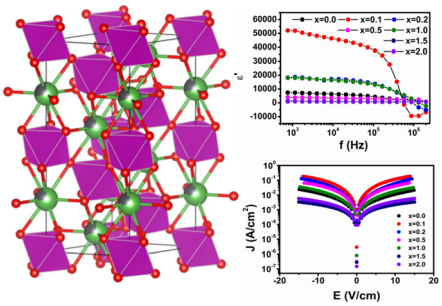

Re-entrant structural phase transition and charge carrier conduction in $La_{2-x}Sr_xFeMnO_6$ solid solutions for electronic device applications

Baniya R. Meena and Anup K. Ghosh*

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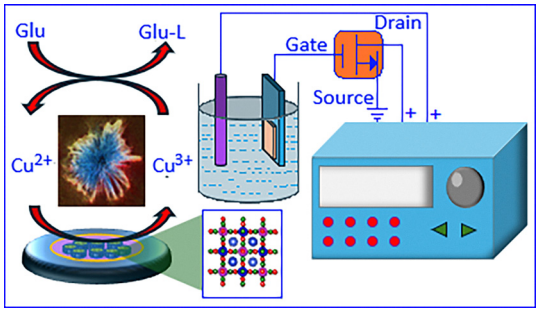
Complexation-driven synthesis of potassium copper ferrocyanide nanoparticles for nonenzymatic glucose detection: an electrochemical and FET-based approach

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



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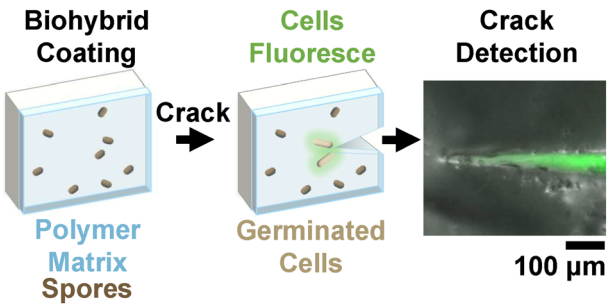
Mechanically driven bacteria-based crack detection

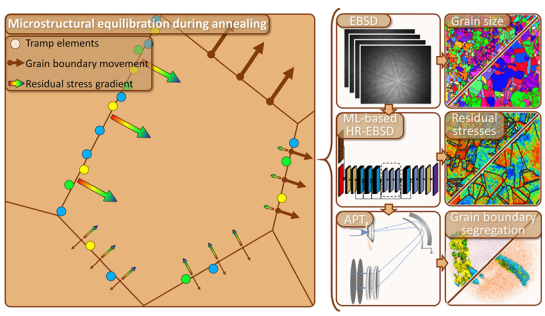
Ellen W. van Wijngaarden, Tyrone Chen, Ilana L. Brito, Nikolaos Bouklas, Andrea Giometto and Meredith N. Silberstein*



1114

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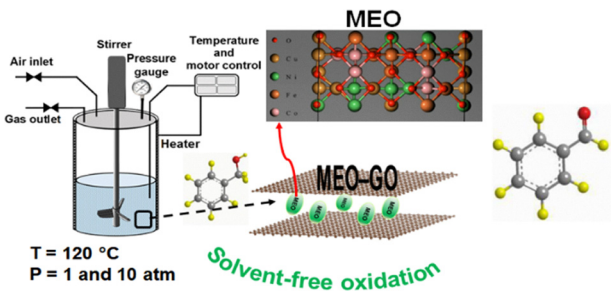
A comparative study of medium-entropy oxide and metal oxide nanoparticles on graphene oxide for benzyl alcohol oxidation under solvent-free conditions

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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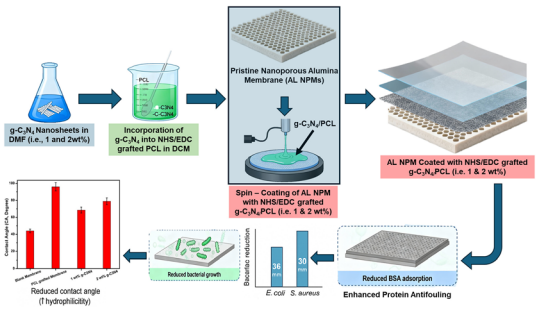

Innovative polycaprolactone/graphitic carbon nitride composite coatings: enhancing the antibacterial properties of nanoporous alumina membranes

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

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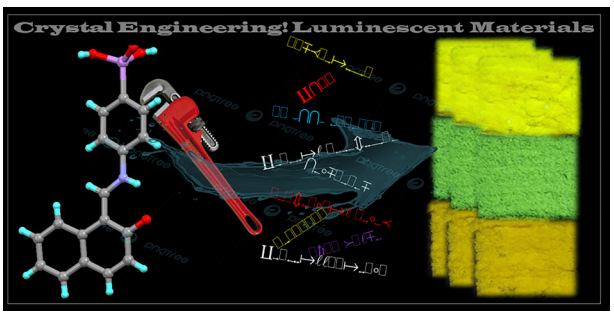

Optical studies of stimuli-responsive organic crystals differing in the position and nature of functional groups

Sumeera Farooq, Ishtiyaq Ahmad and Aijaz A. Dar*

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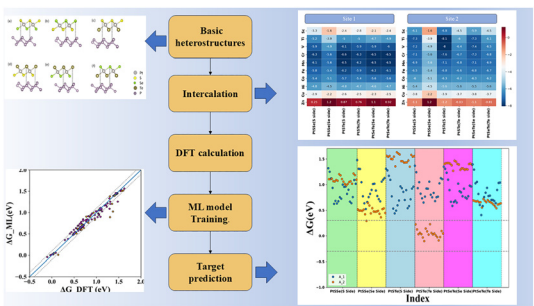

Machine learning screening and high-throughput computation of 3d-transition-metal intercalated Janus PtXY/ζ-phosphorene (X ≠ Y; X, Y = S, Se, Te) heterostructures for photocatalytic water splitting

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

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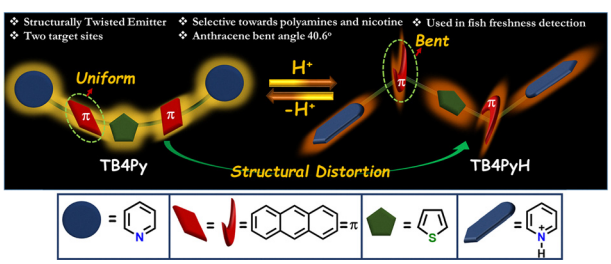

Protonation-driven structural deformation in a conformationally twisted pyridyl-linked AIEgen: a platform to detect polyamines and nicotine

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

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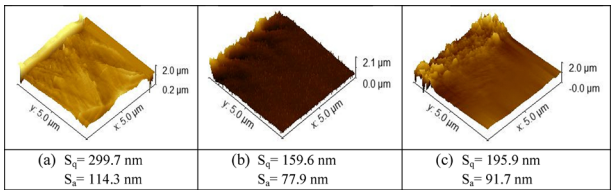
1188

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

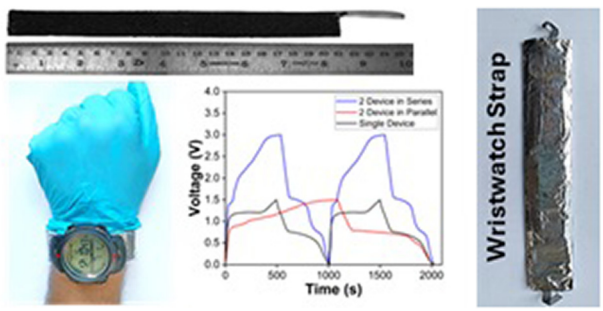
Uzoma Charles Chukwuma,* Joan Ijeoma Arimanwa, Kanayo Lucy Oguzie, Ugochi Nneka Kemka, Ini-Ibehe Nabuk Etim, Sikandar Khan, Kingsley O. Ukaegbu and Emeka Emmanuel Oguzie



1203

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

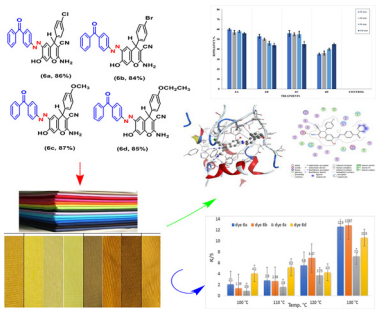
Arunesh Kumar, Arpit Thomas, Michael Lastovich, Bharat Gwalani and Harpreet Singh Arora*



1213

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

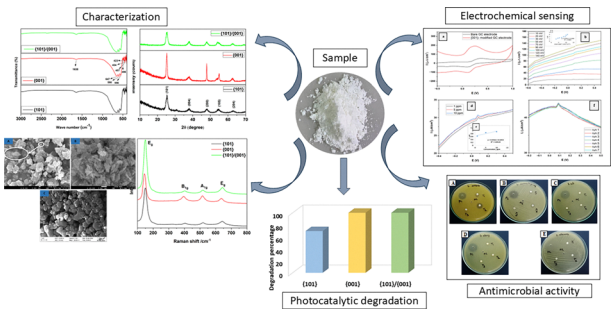
Mohamed S. A. El-Gaby, M. A. Habib, Nadeem Raza, Ahmed B. M. Ibrahim, Ali A. Ali,* Walid E. Elgammal, Ahmed H. Halawa, Mostafa A. Ismail, Tharwat A. Selim, Ahmed I. Hasaballah, Mohamed A. M. El-Tabakh and Gameel A. M. Elhagali



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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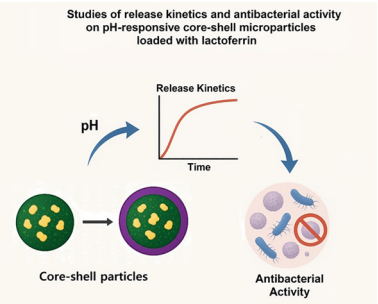
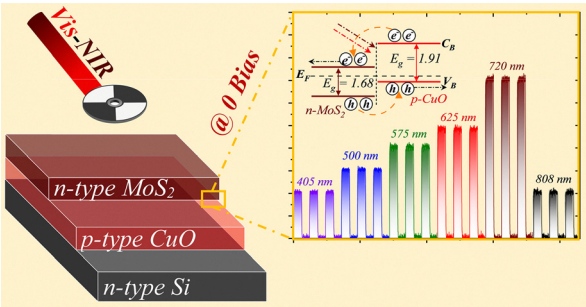
1250



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

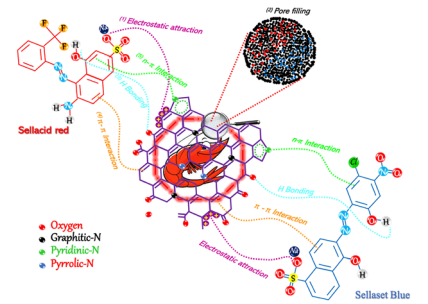
1265



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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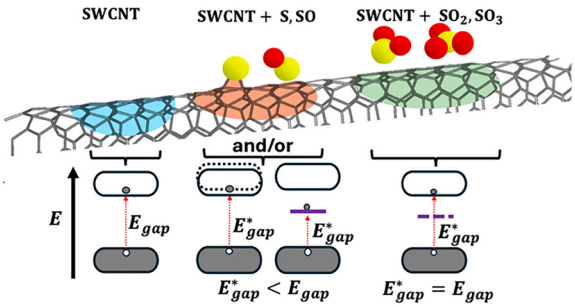
PAPERS

1303

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

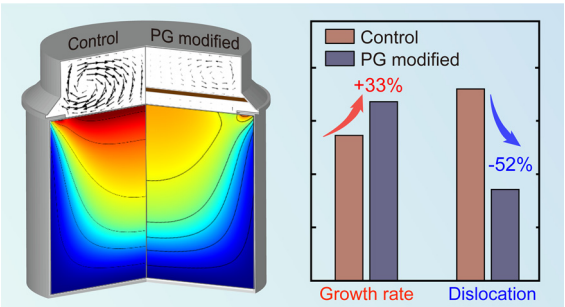
Tina N. Mihm,* Kasidet Jing Trerayapiwat, Xinxin Li, Xuedan Ma and Sahar Sharifzadeh



1311

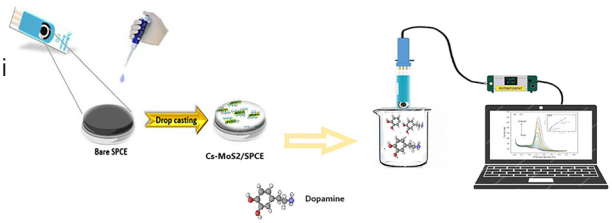
Porous graphite plate design in SiC PVT growth: optimized powder source evolution for enhanced crystal yield and quality

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