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Most popular 2022 physical and theoretical chemistry articles

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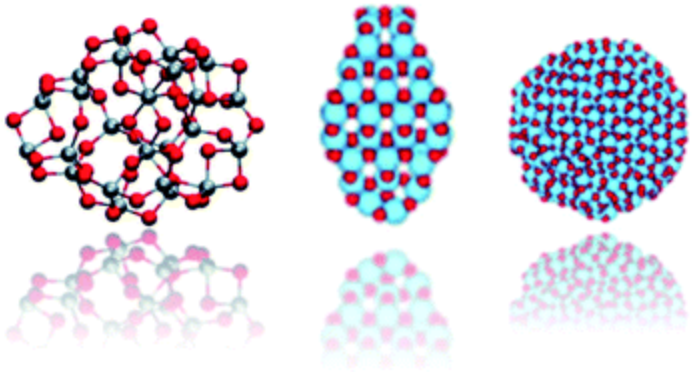
Review Article

Modeling titanium dioxide nanostructures for photocatalysis and photovoltaics

Francesca Nunzi and Filippo De Angelis

The latest findings from theoretical investigations into TiO_2 nanoparticles are reviewed, including both realistic models from a bottom-up approach (1–3 nm diameter) and cut from bulk models (>3 nm diameter) in a top-down approach.



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https://doi.org/10.1039/D2SC02872G

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Review Article

NIR TADF emitters and OLEDs: challenges, progress, and perspectives

Yuxin Xiao, Hailan Wang, Zongliang Xie, Mingyao Shen, Rongjuan Huang, Yuchen Miao, Guanyu Liu, Tao Yu and Wei Huang

This review presents the recent progress of NIR TADF emitters along with their molecular design strategies and photophysical properties, as well as the electroluminescence performance data of the emitters and their OLEDs.

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The article was first published on 11 Jul 2022
Chem. Sci., 2022, **13**, 8906-8923
https://doi.org/10.1039/D2SC02201J

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Edge Article

Data-driven discovery of molecular photoswitches with multioutput Gaussian processes

Ryan-Rhys Griffiths, Jake L. Greenfield, Aditya R. Thawani, Arian R. Jamasb, Henry B. Moss, Anthony Bourached, Penelope Jones, William McCorkindale, Alexander A. Aldrick, Matthew J. Fuchter and Alpha A. Lee

We present a data-driven discovery pipeline for molecular photoswitches through multitask learning with Gaussian processes. Through subsequent screening, we identify several motifs with separated and red-shifted electronic absorption bands.

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The article was first published on 10 Nov 2022
Chem. Sci., 2022, **13**, 13541-13551
https://doi.org/10.1039/D2SC04306H

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Interrogating the thionium hydrogen bond as a noncovalent stereocontrolling interaction in chiral phosphate catalysis

Junshan Lai and Jolene P. Reid

Transferable selectivity profiles allow data from intermolecular reactions using iminium substrates to be applied to predict intramolecular reactions involving thioniums.

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The article was first published on 16 Aug 2022
Chem. Sci., 2022, **13**, 11065-11073
https://doi.org/10.1039/D2SC02171D

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Molecular mechanism of a large conformational change of the quinone cofactor in the semiquinone intermediate of bacterial copper amine oxidase

Mitsuo Shoji, Takeshi Murakawa, Shota Nakanishi, Mauro Boero, Yasuteru Shigeta, Hideyuki Hayashi and Toshihide Okajima

The large conformational change of topaquinone in bacterial copper amine oxidase occurs through the TPQ ring rotation and slide, which are essential to stabilize the semiquinone form.

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The article was first published on 23 Aug 2022
Chem. Sci., 2022, **13**, 10923-10938
https://doi.org/10.1039/D2SC01356H

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Bare and ligand protected planar hexacoordinate silicon in $SiSb_3M_3^+$ (M = Ca, Sr, Ba) clusters

Chen Chen, Meng-hui Wang, Lin-Yan Feng, Lian-Qing Zhao, Jin-Chang Guo, Hua-Jin Zhai, Zhong-hua Cui, Sudip Pan and Gabriel Merino

The global minimum of $SiSb_3M_3^+$ (M = Ca, Sr, Ba) is a D_{3h} symmetric structure containing an elusive planar hexacoordinate silicon (phSi) atom. Most importantly, the phSi core remains intact in ligand protected environment as well.

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$[Cu_{18}H_3(S\text{-}Adm)_{12}(PPh_3)_4Cl_2]$: fusion of Platonic and Johnson solids through a Cu(0) center and its photophysical properties

Anish Kumar Das, Sourav Biswas, Vaibhav S. Wani, Akhil S. Nair, Biswarup Pathak and Sukhendu Mandal

An example of a butterfly-like $[Cu_{18}H_3(S\text{-}Adm)_{12}(PPh_3)_4Cl_2]$ cluster with vertex-sharing kernels through a Cu(0) center. Combined experimental and theoretical results correlate its photophysical properties with its unique structural architecture.

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Chem. Sci., 2022, **13**, 7616-7625
https://doi.org/10.1039/D2SC02544B

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Color-tunable persistent luminescence in 1D zinc–organic halide microcrystals for single-component white light and temperature-gating optical waveguides

Bo Zhou and Dongpeng Yan

1D zinc–organic halide microcrystals exhibiting thermally assisted spectral separation of fluorescence and phosphorescence could be used as single-component standard white-light and temperature-gating active waveguides.

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Chem. Sci., 2022, **13**, 7429-7436
https://doi.org/10.1039/D2SC01947G

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A rechargeable molecular solar thermal system below 0 °C

Zhichun Shangguan, Wenjin Sun, Zhao-Yang Zhang, Dong Fang, Zhihang Wang, Si Wu, Chao Deng, Xianhui Huang, Yixin He, Ruzhu Wang, Tingxian Li, Kasper Moth-Poulsen and Tao Li

We demonstrate rationally designed arylazopyrazoles as MOST-PCM that can be circularly charged and discharged below 0 °C with visible light.

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The article was first published on 16 May 2022
Chem. Sci., 2022, **13**, 6950-6958
https://doi.org/10.1039/D2SC01873J

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Predicting reaction conditions from limited data through active transfer learning

Eunjae Shim, Joshua A. Kammeraad, Ziping Xu, Ambuj Tewari, Tim Cernak and Paul M. Zimmerman

Transfer learning is combined with active learning to discover synthetic reaction conditions in a small-data regime. This strategy is tested on cross-coupling reactions from a high-throughput experimentation dataset and shows promising results.

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The article was first published on 11 May 2022
Chem. Sci., 2022, **13**, 6655-6668
https://doi.org/10.1039/D1SC06932B

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The oxidation state in low-valent beryllium and magnesium compounds

Martí Gimferrer, Sergi Danés, Eva Vos, Cem B. Yildiz, Inés Corral, Anukul Jana, Pedro Salvador and Diego M. Andrada

This article examines the electronic structure of group 2 (E = Be and Mg) ligand stabilized compounds. We elaborate on the donor–acceptor interaction L(0) ⇆ E(0) ⇆ L(0) and diradical L(−1) → E(+2) ← L(−1) pictures to assess the oxidation state of the metal.

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Why heterogeneous single-atom catalysts preferentially produce CO in the electrochemical CO_2 reduction reaction

Yu Wang, Tianyang Liu and Yafei Li

This report discloses a nontrivial role of the CO_2 adsorption mode in governing the CO/formate selectivity of single-atom catalysts towards two-electron CO_2 reduction.

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The article was first published on 04 May 2022
Chem. Sci., 2022, **13**, 6366-6372
https://doi.org/10.1039/D2SC01593E

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Non-covalent reconfigurable microgel colloidosomes with a well-defined bilayer shell

Xin Guan, Yang Liu, Zhili Wan, Ying-Lung Steve Tse and To Ngai

Inverse W/O Pickering emulsions and reconfigurable microgelsomes with a well-defined bilayer structure are prepared from octanol-swollen PNIPAM-*co*-MAA microgels and the combination of binary microgels, which promise wider application of soft colloids.

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Prediction and realisation of high mobility and degenerate p-type conductivity in CaCuP thin films

Joe Willis, Ivona Bravić, Rekha R. Schnepf, Karen N. Heinselman, Bartomeu Monserrat, Thomas Unold, Andriy Zakutayev, David O. Scanlon and Andrea Crovetto

We synthesize air-stable, p-type CaCuP thin films with high hole concentration and high hole mobility as potential p-type transparent conductors. We study their optoelectronic properties in detail by advanced experimental and computational methods.

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Chem. Sci., 2022, **13**, 5872-5883
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Extending conceptual DFT to include external variables: the influence of magnetic fields

Robin Francotte, Tom J. P. Irons, Andrew M. Teale, Frank de Proft and Paul Geerlings

An extension of conceptual DFT to include the influence of an external magnetic field is proposed in the context of a program set up to cope with the ever increasing variability of reaction conditions and

concomitant reactivity.

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https://doi.org/10.1039/D1SC07263C

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Predicting biomolecule adsorption on MoS_2 nanosheets with high structural fidelity

Le Nhan Pham and Tiffany R. Walsh

Benchmarked van der Waals density functional theory calculations are used to create a force-field to describe biomolecule interactions at the aqueous MoS_2 interface, which can recover interfacial biomolecule adsorption with high structural fidelity.

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Chem. Sci., 2022, **13**, 5186-5195
https://doi.org/10.1039/D1SC06814H

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An open source computational workflow for the discovery of autocatalytic networks in abiotic reactions

Aayush Arya, Jessica Ray, Siddhant Sharma, Romulo Cruz Simbron, Alejandro Lozano, Harrison B. Smith, Jakob Lykke Andersen, Huan Chen, Markus Meringer and Henderson James Cleaves

We present an open-source chemoinformatic workflow to generate and analyze complex abiological chemical networks to discover novel compounds and autocatalytic processes. We demonstrate this pipeline's capabilities against a well-studied model system.

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The article was first published on 23 Mar 2022
Chem. Sci., 2022, **13**, 4838-4853
https://doi.org/10.1039/D2SC00256F

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Data-driven discovery of cardiolipin-selective small molecules by computational active learning

Bernadette Mohr, Kirill Shmilovich, Isabel S. Kleinwächter, Dirk Schneider, Andrew L. Ferguson and Tristan Bereau

We present a data-driven approach combining deep learning-enabled active learning with coarse-grained simulations and alchemical free energy calculations to discover small molecules to selectively permeate cardiolipin membranes.

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Chem. Sci., 2022, **13**, 4498-4511
https://doi.org/10.1039/D2SC00116K

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Mining anion–aromatic interactions in the Protein Data Bank

Emilia Kuzniak-Glanowska, Michał Glanowski, Rafał Kurczab, Andrzej J. Bojarski and Robert Podgajny

The comprehensive analysis of non-redundant PDB macromolecular structures investigating anion distributions around all aromatic molecules in available biosystems is presented.

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Model agnostic generation of counterfactual explanations for molecules

Geemi P. Wellawatte, Aditi Seshadri and Andrew D. White

Generating model agnostic molecular counterfactual explanations to explain model predictions.

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https://doi.org/10.1039/D1SC05259D

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Computationally driven discovery of SARS-CoV-2 M^{pro} inhibitors: from design to experimental validation

Léa El Khoury, Zhifeng Jing, Alberto Cuzzolin, Alessandro Deplano, Daniele Loco, Boris Sattarov, Florent Hédin, Sebastian Wendeborn, Chris Ho, Dina El Ahdab, Theo Jaffrelot Inizan, Mattia Sturlese, Alice Sosic, Martina Volpiana, Angela Lugato, Marco Barone, Barbara Gatto, Maria Ludovica Macchia, Massimo Bellanda, Roberto Battistutta, Cristiano Salata, Ivan Kondratov, Rustam Iminov, Andrii Khairulin,

Yaroslav Mykhalonok, Anton Pochepko, Volodymyr Chashka-Ratushnyi, Iaroslava Kos, Stefano Moro, Matthieu Montes, Pengyu Ren, Jay W. Ponder, Louis Lagardère, Jean-Philip Piquemal and Davide Sabbadin

The dominant binding mode of the QUB-00006-Int-07 main protease inhibitor during absolute binding free energy simulations.

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https://doi.org/10.1039/D1SC05892D

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PIGNet: a physics-informed deep learning model toward generalized drug–target interaction predictions

Seokhyun Moon, Wonho Zhung, Soojung Yang, Jaechang Lim and Woo Youn Kim

PIGNet, a deep neural network-based drug–target interaction model guided by physics and extensive data augmentation, shows significantly improved generalization ability and model performance.

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A reactivity model for oxidative addition to palladium enables quantitative predictions for catalytic cross-coupling reactions

Jingru Lu, Sofia Donnecke, Irina Paci and David C. Leitch

We report a quantitative model for oxidative addition reactivity in palladium-catalyzed cross-coupling, which is broadly applicable to predict reactivity and selectivity for complex substrates from simple molecular descriptors.

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Synaptotagmin-1 C2B domains cooperatively stabilize the fusion stalk *via* a master-servant mechanism

Ary Lautaro Di Bartolo and Diego Masone

Synaptotagmin-1 is a low-affinity Ca^{2+} sensor that triggers synchronous vesicle fusion.

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Chem. Sci., 2022, **13**, 3437-3446
https://doi.org/10.1039/D1SC06711G

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Generating 3D molecules conditional on receptor binding sites with deep generative models

Matthew Ragoza, Tomohide Masuda and David Ryan Koes

We generate 3D molecules conditioned on receptor binding sites by training a deep generative model on protein–ligand complexes. Our model uses the conditional receptor information to make chemically relevant changes to the generated molecules.

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https://doi.org/10.1039/D1SC05976A

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Photosensitization mechanisms at the air–water interface of aqueous aerosols

Marilia T. C. Martins-Costa, Josep M. Anglada, Joseph S. Francisco and Manuel F. Ruiz-López

First-principles molecular dynamics simulations of imidazole-2-carboxaldehyde at the air–water interface highlight the role of surfactants in stabilising the reactive triplet state involved in photosensitisation reactions in aqueous aerosols.

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Chem. Sci., 2022, **13**, 2624-2631
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Equilibria between conformational states of the Ras oncogene protein revealed by high pressure crystallography

Eric Girard, Pedro Lopes, Michael Spoerner, Anne-Claire Dhaussy, Thierry Prangé, Hans Robert Kalbitzer and Nathalie Colloc'h

The equilibria between structural states induced by pressure within the crystal structure of Ras are illustrated with different colors corresponding to different Ras substates.

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Low-energy electron distributions from the photoionization of liquid water: a sensitive test of electron mean free paths

Titouan Gadeyne, Pengju Zhang, Axel Schild and Hans Jakob Wörner

Our study reveals the detailed influence of elastic and inelastic mean-free paths on the complete photoelectron spectra of liquid water, including the low-energy electron distributions and the reshaping of the primary photoelectron bands.

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Improving machine learning performance on small chemical reaction data with unsupervised contrastive pretraining

Mingjian Wen, Samuel M. Blau, Xiaowei Xie, Shyam Dwaraknath and Kristin A. Persson

Contrastive pretraining of chemical reactions by matching augmented reaction representations to improve machine learning performance on small reaction datasets.

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MGraphDTA: deep multiscale graph neural network for explainable drug–target binding affinity prediction

Ziduo Yang, Weihe Zhong, Lu Zhao and Calvin Yu-Chian Chen

MGraphDTA is designed to capture the local and global structure of a compound simultaneously for drug–target affinity prediction and can provide explanations that are consistent with pharmacologists.

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Spotlight