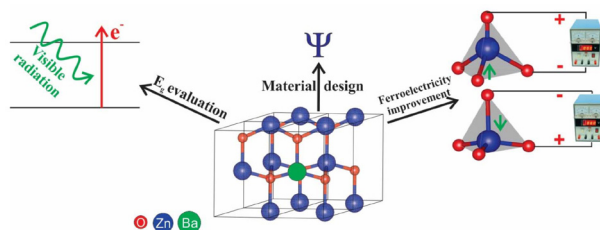


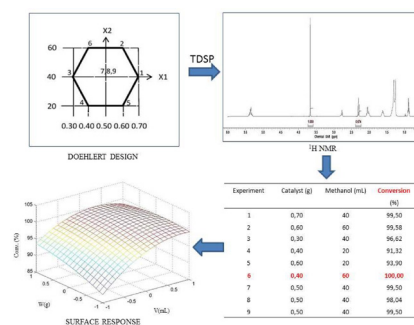
- 261 Ba-DOPED ZnO materials: a DFT simulation to investigate the doping effect on ferroelectricity
Luis H. da S. Lacerda e Sergio R. de Lazaro

The ferroelectric, optical and structural properties of Ba-doped ZnO materials were evaluated through DFT/B3LYP simulations. Results indicate that the Ba doping improves the ferroelectric properties and causes the band gap reduction of ZnO materials.



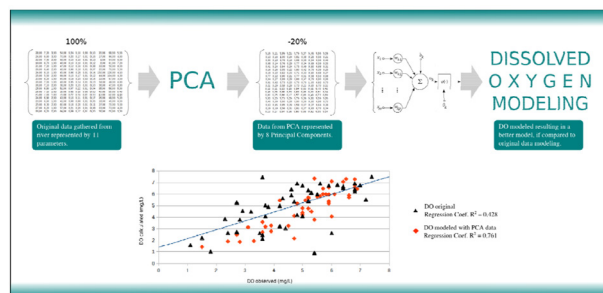
- 267 Otimização do processo de transesterificação em duas etapas para produção de biodiesel através do planejamento experimental Doehlert
Carla F. C. Ruschel, Marco F. Ferrão, Francisco P. Dos Santos e Dimitrios Samios

Biodiesel was produced by TDSP methodology employing Doehlert experimental design. The results were evaluated by surface response and by RMN ^1H was obtained conversion values that were interpreted to define what the best parameters of optimization of transesterification reaction.



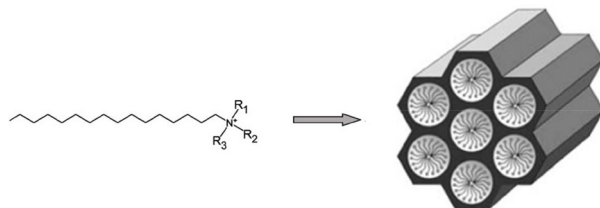
- 273 Redução de variáveis de entrada de redes neurais artificiais a partir de dados de análise de componentes principais na modelagem de oxigênio dissolvido
Saulo R. e Silva e Fernando Schmidt

The original data is reduced by 20%, after processed in PCA, being then represented by 8 Principal Components. The Dissolved Oxygen modeled as from this data results in a better model, if compared to the original.

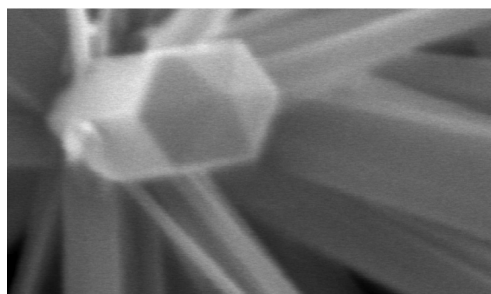


- 279 Síntese e propriedades de sílicas híbridas contendo surfactantes cetiltrialquilamônio
Ana F. P. de Campos, Aurélia R. O. Ferreira e Dilson Cardoso

The graphical abstract represents the hybrid mesoporous silicas containing cetyltrialquilammonium surfactants.

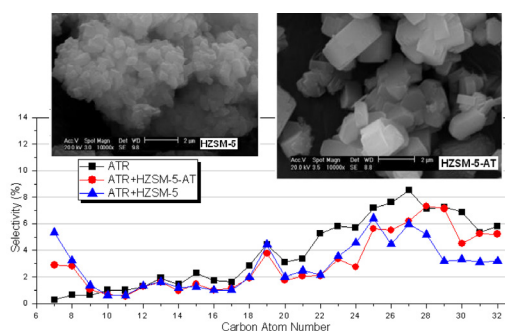


- 286 Obtaining ZnO immobilized over different substrates by hydrothermal treatment for photocatalysis application
Mônica Bagnara, Jéssica Farias and Marla A. Lansarin



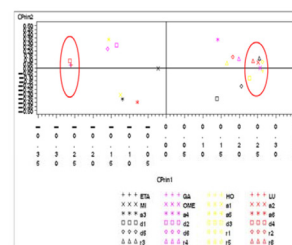
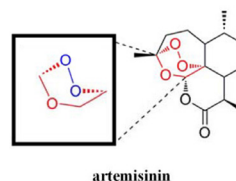
The synthesis of zinc oxide nanorods on three different substrates was studied. A design of experiments was used to investigate the effect of synthesis variables on morphology and photocatalytic activity of samples.

- 292 Use of a low-cost template-free ZSM-5 for atmospheric petroleum residue pyrolysis
Vinícius P. S. Caldeira, Anne G. D. Santos, Sibele B. C. Pergher, Maria J. F. Costa and Antonio S. Araujo



On Graphical Abstract demonstrated in the micrographs of both zeolites and the distribution by carbon atom number obtained during the pyrolysis of ATR over ZSM-5 samples.

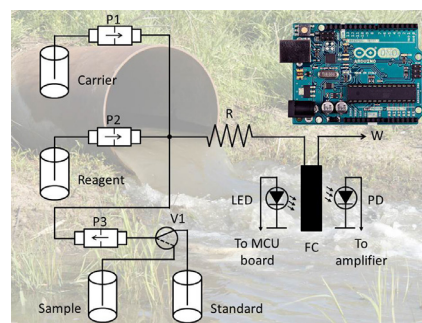
- 298 Comparação entre funcionais de densidade no estudo de propriedades eletrônicas de derivados da artemisinina
Victor H. S. C. Batista, Ana C. Granato e Wagner F. D. Angelotti



Electronic variable of artemisinin in the first factorial plan

Multivariate Principal Component Analysis was used to study the artemisinin and two derivatives that were computational analyzed by density functions contained in GAMESS.

- 305 Low cost analyzer for the determination of phosphorus based on open-source hardware and pulsed flows
Pablo González, Nicolás Pérez and Moisés Knochen

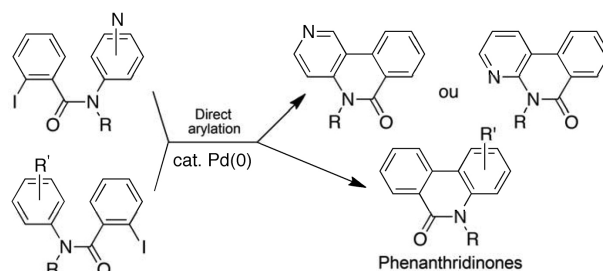


Use of a pulsed-flow system under control of open-source microcontroller board allows determination of soluble phosphorus levels in levels in industrial samples and effluents.

9

- 310 Síntese de derivados de fenantridinonas por arilação direta. Caracterização dos espectros de absorção e emissão de exemplos representativos

Roberta L. da Costa, Douglas A. F. da Silva, Nanci C. de Lucas e Simon J. Garden

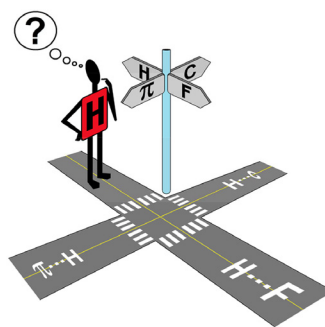


Examples of phenanthridinones were prepared by palladium catalyzed direct arylation and the absorption and emission spectra of selected examples were characterized.

10

- 320 A formação de ligações de hidrogênio $\pi \cdots \text{H}$, $\text{F} \cdots \text{H}$ e $\text{C} \cdots \text{H}$ nos complexos $\text{C}_2\text{H}_2 \cdots (\text{HF})$, $\text{C}_2\text{H}_2 \cdots 2(\text{HF})$ e $\text{C}_2\text{H}_2 \cdots 3(\text{HF})$

Boaz G. Oliveira



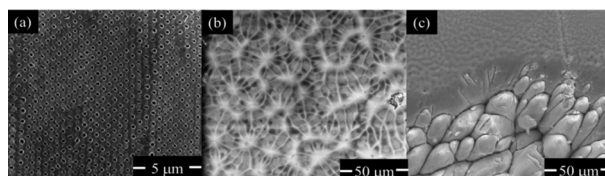
Different proton receptors and the possibility to form the $\pi \cdots \text{H}$, $\text{F} \cdots \text{H}$ e $\text{C} \cdots \text{H}$ hydrogen bonds on the $\text{C}_2\text{H}_2 \cdots (\text{HF})$, $\text{C}_2\text{H}_2 \cdots 2(\text{HF})$ and $\text{C}_2\text{H}_2 \cdots 3(\text{HF})$ complexes.

Revisão

11

- 328 Materiais vítreos e luz: parte 1

Marcelo Nalin, Sidney J. L. Ribeiro, Danilo Manzani, Rogéria R. Gonçalves, Gael Poirier, Fabia C. Cassanges, Christiano J. S. de Matos, Cleber R. Mendonça, Leonardo de Boni, Lino Misoguti, Oscar Malta, Yannick Ledemi, Sandra Messaddeq e Younes Messaddeq

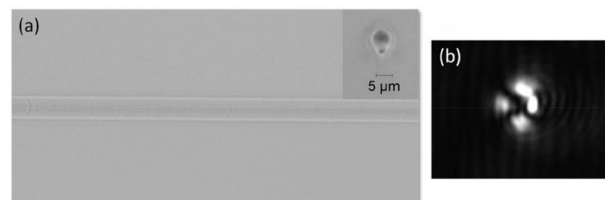


Different kinds of structures produced by interaction of fs-laser with chalcogenide glasses having different bandgaps (a) $\text{Ge}_{20}\text{S}_{80}$, (b) $\text{Ge}_{20}\text{Se}_{80}$ e (c) $\text{Ge}_{20}\text{Te}_{80}$.

12

- 340 Materiais vítreos e luz: parte 2

Marcelo Nalin, Sidney J. L. Ribeiro, Danilo Manzani, Rogéria R. Gonçalves, Gael Poirier, Fabia C. Cassanges, Christiano J. S. de Matos, Cleber R. Mendonça, Leonardo de Boni, Lino Misoguti, Oscar Malta, Yannick Ledemi, Sandra Messaddeq e Younes Messaddeq



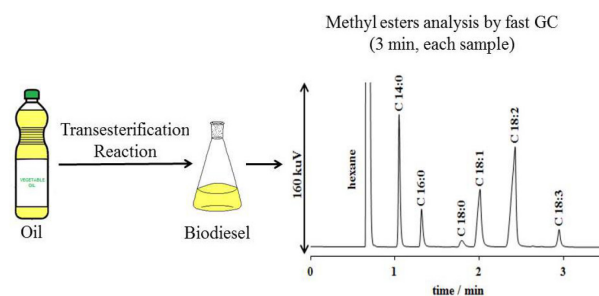
a) Optical microscopy of a waveguide obtained in a glass using fs-laser. b) Light profile from the output signal of the waveguide at 632.8 nm.

Nota Técnica

- 13 352 Fast GC-FID method for monitoring acidic and basic catalytic transesterification reactions in vegetable oils to methyl ester biodiesel preparation

Renata T. Sato, Pedro H. F. Stroppa, Adilson D. da Silva, Marcone A. L. de Oliveira

An alternative method, by fast GC-FID, was proposed to analyze fatty acid methyl esters in different biodiesel samples, obtained by acid or basic catalysis transesterification reactions.

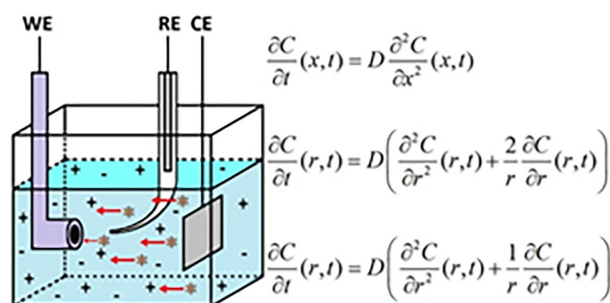


Educação

- 14 356 Compreensão matemática da difusão no contexto eletroquímico

Sidineia Barrozo e Assis V. Benedetti

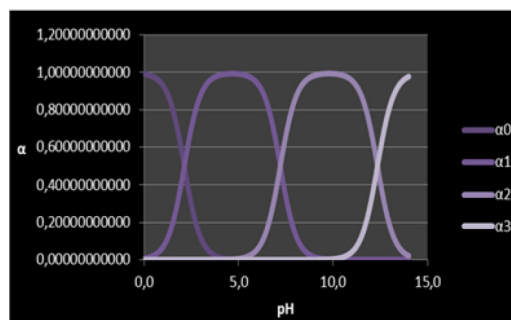
Diffusion equations in electrochemistry without mysteries: understanding their deductions and resolutions in all the mathematical details in a charge transfer process.



- 15 371 Avaliação do uso de planilhas computacionais como uma ferramenta didática em Química Analítica Qualitativa

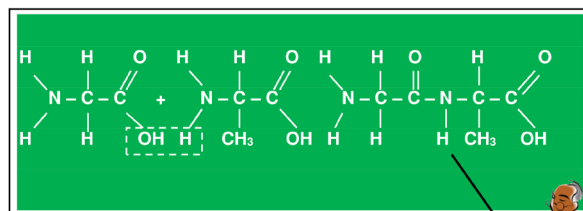
Gabriela B. Denari, Thalita R. Saciloto e Éder T. G. Cavalheiro

Typical result from the use of the spreadsheet software by the students, representing the fraction of phosphoric acid species as a function of pH.



- 16 376 O conhecimento pedagógico dos docentes de química do ensino superior

Cátia S. F. Primon e Agnaldo Arroio



Knowledge of teaching chemistry of higher education teachers.

- 17 383 Casos investigativos e a relação com o saber: trajetória e processo de aprendizagem de estudantes do ensino superior no Tocantins

Wellington Francisco e Anna M. C. Benite

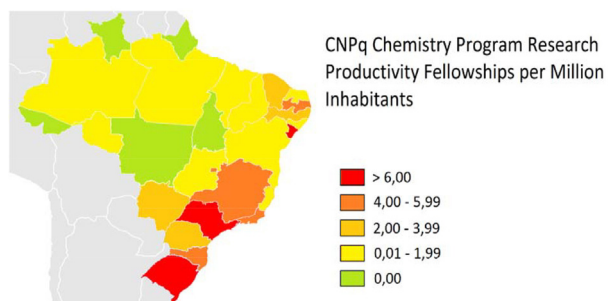


The trajectories for the resolution of the case and the chemistry learning are influenced by different relationships with knowledge that they can be relationship with the world, relationship with others and relationship with yourself.

Assuntos Gerais

- 18 393 Perfil dos bolsistas de produtividade em pesquisa nas subáreas da química do CNPq

Lucilene F. O. Cândido, Natacha C. F. Santos e João B. T. da Rocha



Chemistry, its specialties and specificities in research productivity.

Carta ao Editor

- 19 406 Henry Taube centenary – Some remarks of a great scientist in Brazil

Henrique E. Toma

