The Topology Impact Hydrogen Storage Capacity Y-Decorated on Porous Graphene

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Abstract

Hydrogen storage capacity of yttrium (Y)-decorated on porous graphene (PG) was examined through density functional theory calculations. PGs were selected considering topological symmetries. Our calculations show that the most stable locations for adsorption of Y are located on the center of carbon rings and the polarization and the hybridization mechanisms both contribute to the Y atom adsorption on PGs. Analysis of charge density difference demonstrated that the presence of Y could play an efficient role for stronger adsorption of hydrogen molecules rather than increasing pore sizes. Compared to H2 adsorption on graphene, injecting topological defect such as hexagon porous and decoration with a transition metal atom such as Y can effectively create much more conductive states at Fermi energy. A maximum of four hydrogen molecules can be adsorbed on Y-PGs system. The highest average adsorption energy is related to porous graphene with larger pore size with average absorption energies of 0.513 eV.

Keywords: Porous Graphene, Hydrogen Storage, Y-Decorated, Plane Wave.

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Comparison of Artificial Neural Network and Different Mathematical Models for Estimation of Moisture Rate in Quince Fruit Drying

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Abstract

In this research, the process of drying the quince fruit and the effect of various parameters such as the drying air speed, time, temperature and thickness on moisture ratio were studied. 7 mathematical models were fitted to the data obtained from 27 series of experiments and the best model was selected. Modeling was also performed by artificial neural network. In this modeling, the effect of all input parameters on the drying process was investigated simultaneously. The selective network structure was considered multi-layer perceptron with the back-propagation algorithm. By researching the number of different hidden layer neurons and different transfer functions, 9 neurons and "logsig" transfer function were used for the hidden layer and "purelin" transfer function for the output layer. Modeling by artificial neural network predicted the simultaneous effect of the four input parameters with very high accuracy. The results showed that ANN modeling had better accuracy than the best mathematical model.

Keywords: Artificial Neural Network, Moisture Ratio, Mathematical Model.

Study and Investigation of Process Parameters for Solvent Extraction of Cobalt from Chloride Solution by Using Mixture of Compelxing Agents Cyanex272, TBP, TOPO

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Abstract

In this study, the process of cobalt extraction from chloride solution was investigated by using a mixture of TBP, TOPO and Cyanex272 extractants. Process parameters such as the effect of aqueous solution of pH, extractant concentrations, aqueous to organic phase ratio and the stripping with different acids in cobalt extraction were investigated. The results showed that the obtained mixture from TBP, TOPO and Cyanex272 extractants with concentrations of 0.2, 0.1 and 0.3 mol/l, respectively, is suitable for the optimal extraction of cobalt with an extraction efficiency above 91.39%. Sulfuric acid with a concentration of one mole per liter was used as a suitable reagent in the recovery stage with the stripping percent of over than 99.2%. In this study, a mixed synergistic system was reported that is very effective in separation of metal ions and can be used in the recovery of lithium batteries by hydrometallurgical method.

Keywords: Cobalt, Solvent Extraction, Synergistic, Operating Parameter, Mixture of Extractants.

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Experimental Modeling of CO_2 Absorption into Monoethanolamine Amine Using Response Surface Methodology

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Abstract

Carbon dioxide gas is one of the main environmental pollutants that can cause irreparable damage by changing the climate, so solving this problem requires serious attention. Chemical absorption of CO_2 with alkanoamine aqueous solutions is currently the most common commercial method of high-efficiency separation in the industry. Among the various methods of removing carbon dioxide from flue gases, the monoethanolamine (MEA) aqueous solvent absorption process has been the most important option for industrial applications in recent years. In this research, MEA solvent has been used to evaluate the amount of CO_2 absorption. The experimental range of the studied parameters includes temperature of 20-60 C, pressure of 3.5-9.5 bar and solvent concentration of 2.5-8.5% w. Loading and CO_2 absorption percent in MEA aqueous solution were obtained in the range of 0.70-2.615 and 17.81-48.65%, respectively. To analyze the results, the quadratic polynomial model using the response surface method (RSM) has been used. Numerical optimization has also been used to find the maximum loading and absorption percent under optimal conditions. Under optimal conditions, the maximum loading and absorption percent are estimated to be 0.552 and 44.17%, respectively.

Keywords: Absorption, CO_2, Monoethanolamine, Response Surface Methodology (RSM).

A Review of DNA Purification Methods: Microfluidics Systems

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Abstract

Because of the importance of biomolecule extraction and its genetic investigations in the medical and forensic field with all the limitations such as sensitivity, nature of work, high cost, the need for highly skilled technicians, automation and portability of the system in terms of detection with existing technologies, several need not fulfilled. There is a need to integrate sample preparation and detection methods. To overcome these limitations, nowadays most studies have focused on improving detection technologies, and accordingly, advances in detection technologies microfluidics is one of the best systems with convincing feautures. Other advantages of this technology including the extraction of DNA and protein which is involved automation in a sample preparation, the ability to operate in small sample sizes as well as minimizing the consumption, cost, and processing time of solvents.

Keywords: Microfluidics, Biomolecules, DNA, Protein.

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Investigation of Methods and Affecting Factors on the Synthesis of Copper (I) Oxide Nanoparticles in Stable Form

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Abstract

In recent years, monovalent copper oxide (Cu_2O) nanoparticles have been used in various industries due to their unique properties. Due to its importance and many applications, common methods of synthesis of these nanoparticles, which are usually done by chemical reduction and sedimentation in an alkaline aqueous medium, have been studied in four groups: precipitation, solvothermal/ hydrothermal, sonochemical and electrochemical. Properties, stability, as well as the performance of this nanoparticle depends on how it is made and the parameters that affect its size, structure, shape, purity and stability. Therefore, the effect of factors such as type of surfactant and precursor, coating and reducing agent, temperature and reaction time, stirring speed of raw materials and concentration of solvent used has been investigated. By increasing the reducing agent concentration, stirring speed, precursor and solvent concentrations to the optimum, the size of the synthetic particles will be smaller.

Keywords: Copper (I) Oxide, Precipitation, Hydrothermal.