MS16-P26

Revisesd Jiang model's «New formula of Prediction of lattice constant in cubic perovskites»

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ABX_3 Perovskite materials are of great interest in the new technology because of the possibility of modifying their physical properties by numerous ionic substitutions.

The mesh parameter prediction model used is useful for providing the predicted structural information for estimating the physical properties of materials for which accurate structural data are not available.

It is also useful as a guide for synthetic exploratory efforts as a starting point for structural characterization improvements of new materials.

Our reformulation of Jiang's model allowed us to obtain a new equation of parameter prediction of cubic perovskite structures taking into account 158 materials.

The results obtained are in good agreement with the experimental with a relative error of the order of 2.64%.

This prediction equation allowed us to predict the mail parameter of 20 new perovskite oxides.

Keywords: mail parameter prediction, cubic perovskite, tolerance factor.

MS17- Biominerals and bioinspired materials

Chairs: Prof. Wolfgang Schmahl, Dr. Anna Schenk

MS17-P01

Removal of methylene blue by adsorption using modified hydroxyapatite by carrageenan biopolymer

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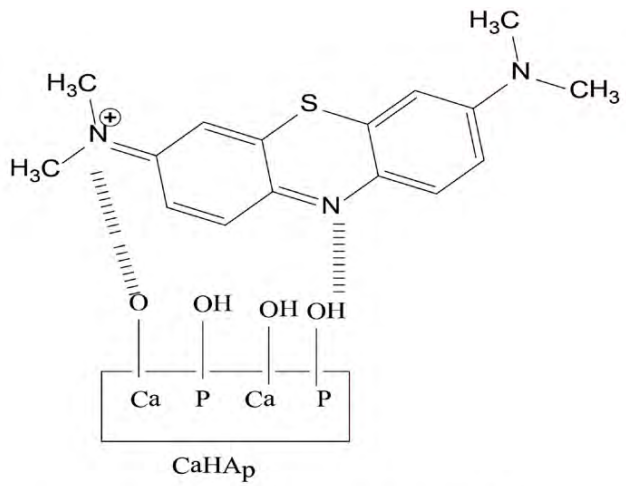
The application of hydroxyapatite modified by biopolymers for the immobilization of various pollutants has been considered as a promising pollution control technology. In this scope, hydroxyapatite-Lambda carrageenan CaHAp-(λ-Carr) hybrid materials were prepared by co-precipitation method with different content of the bio-polymer (0, 5, 10 and 20%). Synthesized materials were characterized using X-ray diffraction (XRD), Infrared spectroscopy (FT-IR), chemical analysis, Scanning Electron Microscopy (SEM), specific surface area (SS) and pH_{zpc} measurement. The X-ray powder analysis showed that the cristallinity is affected by the presence of the biopolymer. The FT-IR spectra show the presence of (λ-Carr) and CaHAp characteristic vibrations in the resulting product. After grafting BET measurements yielded particle specific surface areas ranging from 93 to 260 $m^2\ g^{-1}$ depending on the grafted biopolymer. The adsorption capacities of methylene blue (MB) were investigated with respect to the effect of adsorbent amount, pH value, contact time, adsorbent dose, temperature and initial dye concentration. The pseudo-second-order and Freundlich isotherm equations were found to describe the adsorption mechanism. The percentage of MB removal by CaHAp and CaHAp-(λ-Carr)10 were equal to 81.40 % and 95.63 %, respectively. The results indicate that the modified hydroxyapatite possessed good adsorption ability towards MB dye and can be used as a low cost adsorbent for dye removal from wastewater.



The possible mode of interaction between **MB** dye and **CaHAp** surface.

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Keywords: Hydroxyapatite, Biopolymer, Adsorption.

MS17-P02

Small-angle X-ray scattering studies on the self-assembly of disc shaped bicelles with DNA

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Disc-shaped bicelles can be formed spontaneously by mixing long-chain lipids with short-chain lipids at suitable ratios. The long-chain lipids form the bilayer core of the bicelle while the short-chain lipids form the protecting rim of the bicelle. The typical mixed lipid bicelles have a relatively uniform diameter around 20 nm. The surface charge of such bicelles can be varied by doping with cationic lipids to form cationic bicelles (CB) or with anionic lipids to form anionic bicelles (AB). Different from the typical method of encapsulating DNA with liposomes, bicelles can also be used to form cationic or anionic bicelle-DNA complexes [1-3], which can be used as nonviral vectors for improving the transfection efficiency of gene therapy. As revealed by small-angle X-ray scattering and TEM, one-dimensional alternating stacks of disc cationic bilayer plates (bicelles) and DNA arrays were formed spontaneously. DNA molecules encapsulated between the disc bilayer plates form ordered arrays with a spacing around 4~5 nm. The number of the stacking layers can be easily tuned from just a few stacks to more than one hundred stacks by adjusting the doping percentage of the cationic lipid. It is also possible to form anionic bicelle-DNA complexes with the help of the divalent cations. The DNA-ion-disk bilayer complexes are formed in the investigated range of 10 mM to 100 mM calcium ion concentrations. Other than using short-chain lipids, it was found that bicelles can also be formed at a Triton X-100 to DPPC molar ratio around 1 to 2. As compared with the diC7PC/DPPC bicelle, which can be formed for a diC7PC to DPPC molar ratio around 0.2 to 1, it seems that it takes more Triton X-100 than the short-chain lipid to form bicelles for a fixed amount of DPPC. The prepared DPPC/Triton X-100 cationic bicelles were also found to be able to form complexes with DNA.

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Keywords: bicelle, small-angle X-ray scattering, DNA encapsulation