

mechanisms implying periplasmic protein activity (e.g. alkaline phosphatase) and metabolic activity (e.g. sulfate reducing bacteria) will be reviewed.

**Keywords:** biomineralization, carbonate formation, polysaccharides

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#### Nano-scale Studies of Processes on Crystal Surfaces in Aqueous Solutions

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At the crystal-water interface a large diversity of processes takes place which influence or even control environmental conditions. Among these processes are sorption, growth, dissolution, formation of surface complexes or metastable phases by leaching, repolymerization, or precipitation. For a detailed understanding of these processes, factors and properties such as the stability of metastable phases or structural frameworks need to be taken into account.

Hydrothermal atomic force microscopy has been used for nano-scale in-situ investigations of crystal surfaces in aqueous solutions [1-3]. The method can provide insights into the molecular mechanisms and kinetics of solid-liquid interface processes. The results stress that especially for processes taking place at silicate-water interfaces the consideration of the stability of metastable states and structural influences is very important. In contrast, mechanisms of processes at interfaces like the carbonate-water interface although largely unsolved rather seem to comprise sequences of less numerous steps.

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**Keywords:** surfaces and interfaces, AFM, silicates

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#### Hydrothermal Preparation of TiO<sub>2</sub>: AC Composite Crystalline Particulates

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A highly active, monodispersed designer crystalline nanoparticulate TiO<sub>2</sub> has been impregnated onto the activated carbon surface under mild hydrothermal conditions (<250°C, P~40 bars) which finds the application as photocatalyst. Conventionally TiO<sub>2</sub> is prepared through solid state reactions, etc; further the hydrothermal impregnation of such particulates onto the surface layers of activated carbon has not been carried out either to. The hydrothermal technique provides an easy and one-step method to obtain monodispersed and well crystallized desired products and also eliminates the high temperature firing or pyrolysis required by the other methods. In the present study various hydrothermal experimental parameters like the starting precursors, mineralizers, temperature, etc., were taken into consideration for the impregnation experiments. The as-prepared catalyst composite was characterized by various techniques like XRD, SEM-EDX, PALS, BET and FTIR. The XRD results showed the persisting nature of anatase phase of TiO<sub>2</sub> deposited on the activated carbon surface. The BET and FTIR results reveal an optimum (TiO<sub>2</sub> to AC ratio) conditions for the impregnation. The PALS results further confirmed that TiO<sub>2</sub> is impregnated onto the surface and wider pores (macro- and mesopores) of the activated carbon and the micropores do not play a significant role as far as the TiO<sub>2</sub> impregnation is

concerned. The results of the study finally revealed that TiO<sub>2</sub> could be effectively impregnated onto the activated carbon surface layers under mild hydrothermal conditions and such a designer crystalline particulate composite is highly useful for the environmental issues such as degradation of hazardous organics/wastes, treatment of effluents, air purification and so on.

**Keywords:** hydrothermal impregnation, photocatalyst, TiO<sub>2</sub>: AC composite

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#### Crystalline Structure of Biodegradable Polyhydroxybutyrate thin Films

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Polyhydroxybutyrate: PHB and random copolymer, Polyhydroxyalkanoates: PHAs are crystalline biodegradable polyesters. As a substitute for petrochemical materials, the study of biodegradable polymer has attracted considerable attention. Our recent study demonstrated that melting behavior of a new random copolymer, Poly(3-hydroxybutyrate-co-3-hydroxyhexanoate): P(3HB-co-3HHx) showed a sharp contrast with that of PHB. A novel intermolecular interaction successfully explained the results.

As a next step, we are now conducting the X-ray reflectivity (XR) and grazing incidence X-ray diffraction (GIXD) measurements of thin films of PHB and P(3HB-co-3HHx) at various temperatures. The aim of this study is to get information on morphology, crystallinity, and crystal structure in the surface and thin films, which must be crucial for understanding the physical properties peculiar to the surface region and the mechanism of bio-degradation on a microscopic standpoint.

Both PHB and P(3HB-co-3HHx) thin films indicated that the crystallites tend to orient their *b*-axis along the surface normal direction. The present results strongly support the intermolecular interaction along the *a*-axis direction, which was suggested by the previous study on bulk samples. According to Bragg reflection from the near-surface region, surface morphology of PHB is different from that of P(3HB-co-3HHx) even at room temperature. We will also discuss the results of FT-IR spectrum obtained from the thin films.

**Keywords:** biodegradable polymer, X-ray diffraction, thin film

## MS94 CRYSTALLOGRAPHIC KNOWLEDGE IN DRUG DESIGN STRATEGIES

**Chairpersons:** Franck Leveiller, Michele Saviano

### MS94.30.1

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#### Can Structures lead to Better Drugs? Lessons from Ribosomal Antibiotics

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Ribosomes, the universal cellular organelles catalyzing the translation of genetic code into proteins, are giant asymmetric riboprotein assemblies with a striking architecture and inherent mobility, enabling their function as ribozymes how place their substrate in stereochemistry suitable for peptide bond formation and substrate mediated catalysis. As the main player in a fundamental cell process, ribosomes are targeted by many antibiotics. Structures of over a dozen antibiotics complexes, obtained by using eubacterial ribosomes suitable to serve as pathogen models at clinically relevant concentrations, showed that although theoretically the giant ribosome offers numerous binding opportunities, ribosomal antibiotics bind to a single or a few binding sites; that most antibiotics interact primarily with ribosomal RNA and cause minor conformational changes; that minute structural differences, scattered in various ribosomal locations, are responsible for antibiotic selectivity; that the properties of the antibiotic-binding modes are dictated by species-specific binding pocket composition and conformation, the functional state of the ribosome, and the drugs chemical nature; that resistance to ribosomal