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RESEARCH AND EDUCATION IN X-RAY CRYSTALLOGRAPHY IN THE PREDOMINANTLY UNDERGRADUATE INSTITUTION

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Some members of the research community view crystal structure analysis as being 'too easy', and they have challenged the value of crystallographic results as being irrelevant beyond the solid state, despite numerous examples to the contrary. Crystallography is a field that borders on many other disciplines, and it provides enabling technology, methodology and information. Crystallography is also a key underpinning of post-genomic science. Crystallography is not so easy and routine that anyone can do it, and do it right. However, with solid experimental (not just theoretical) training in the fundamentals, good crystallography (and accurate molecular models) can be achieved. The W.M. Keck Foundation Center for Molecular Structure (CMolS) at California State University Fullerton is a comprehensive x-ray crystallographic and computational facility located in a predominantly undergraduate institution. CMolS is a core facility of the California State University Program for Research and Education in Biotechnology, where faculty and primarily undergraduate student investigators throughout the 23-campus CSU are engaged in joint research and education activities directed at the determination and critical analysis of both small and macromolecular structures. CMolS has begun to uniquely address a post-genomic workforce demand for individuals suitably trained in x-ray crystallographic methods. Faculty and students may conduct experiments in distant classrooms and laboratories through our remote access data acquisition system, with the ability to access shared data files and laboratory materials in the form of online lab manuals, courseware, interactive tutorials, and reporting templates. at the Fullerton campus, we have developed and implemented x-ray diffraction experiments at all levels of the curriculum. CMolS hosts an annual three-day short course, entitled 'Crystallography for Chemists', which is attended by faculty, graduate students, and members of industry. Our efforts have lead to inspiring collaborations in molecular structure and made possible highly specialized training and research despite local geographical and financial limitations.

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TEACHING THE MECHANISM OF THE EPITAXIAL GROWTH USING THE QUANTUM MECHANICAL APPROACH

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Computer-aided quantum mechanical approach is now a powerful tool for investigating various material properties in the field of crystal growth. The availability of the quantum mechanical approach is demonstrated by exemplifying GaAs epitaxial growth and extracting crucial factor for the growth mechanism. The complicated epitaxial growth processes for GaAs are simplified by considering the number of electrons DZ remaining in the surface Ga dangling bonds. The quantum mechanical calculations imply that the elemental growth processes such as migration, adsorption and desorption energies of Ga and As are simply described as CDZ, where C is constant. According to the simple function of DZ, it is found that the migration, adsorption and desorption processes are promoted by decrease of the DZ resulting from charge transfer from surface Ga to As dangling bonds. This is because the dangling bond energy level of Ga is located in the conduction band, and should, therefore, empty, while that for As is in the valence band and should be filled. The simple criterion is applied to dynamic change in atomic arrangements during GaAs epitaxial growth on various reconstructed surfaces. The simulation results reveal that the epitaxial growth of GaAs is continued by restoring the condition of DZ = 0. The predicted growth processes are experimentally verified by recent STM observations. Consequently, these successful applications suggest that the simplified quantum mechanical approach is useful for teaching the mechanism of the epitaxial growth.

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TEACHING THE PRINCIPLES AND APPLICATIONS OF X-RAY FREE-ELECTRON LASER RADIATION

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The generation of very intense free-electron laser (FEL) radiation using high energy electron accelerators will enable new x-ray scattering applications in many scientific domains. In the wavelength regime from 0.1 nm to 100 nm short-wavelength XFEL radiation will provide 10^{12} - 10^{13} photons per pulse of typically 100 fs duration. Since peak powers in the GW regime and pulse energies of several mJ have been proposed these sources will enter into the high-field domain of optical lasers, yet at unprecedented short wavelength. To generate FEL radiation at short wavelength the principle of self-amplified spontaneous emission (SASE) is applied. Understanding the SASE principle is achieved by looking into the interaction of the co-propagating electro-magnetic wave and the electron pulse, leading to modulation of the electron pulse and initiation of the laser amplification. The properties of the emitted XFEL radiation can be understood analyzing the SASE process. First results, obtained at DESY, Hamburg, allow further a comparison of theoretical calculations and experimental observations. Due to its outstanding properties XFEL radiation will explore new regimes of x-ray science. New experimental techniques, like scattering using coherent x-rays, femtosecond time-resolved x-ray scattering or single-molecule investigations, have been proposed for scientific applications in the biology, chemistry and physics. This impact can be extrapolated from first experimental results obtained at DESY.

Keywords: X-RAY FREE-ELECTRON LASERS, COHERENT X-RAYS, TIME-RESOLVED X-RAY SCATTERING

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TOWARDS 30 YEARS OF CRYSTALLOGRAPHIC TEACHING IN ERICE : OUTCOME AND PROSPECTIVES

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The several facets of gathering crystallographers and related scientists during thirty three interdisciplinary meetings will be presented together with those planned for the future, till 2007. Among a great variety of topics, some 'pillars' of the most promising developments of crystallography, e.g. Direct Methods, Molecular Biology, Theoretical and Materials Chemistry, Pharmaceutical Sciences, have marked periodically the most relevant contributions and the exciting progress within these sciences. Though off the beaten track from most common world laboratories, Erice offers a special atmosphere and the local asset stimulate continuous interactions between younger and senior scientists; it is with some pride that we can report the appointment as present directors and invited speakers of a great number of those who came to Erice for the first time as postgraduates or fresh postdoctoral students. Moreover, quite often crystallographers have anticipated the advantages of the modern information technology, adopted later by the hundred or so fields of science active within the Ettore Majorana Centre. Questionnaires report to the organizers news about enthusiastic satisfaction by the attendees: the staff at the Majorana Centre now declares the crystallographic meetings are the most efficient and successful.

Keywords: ERICE COURSES,PAST,FUTURE