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THE EBI MACROMOLECULAR STRUCTURE DATABASE (E-MSD) AND STRUCTURAL GENOMICS

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High throughput structural genomics projects are now underway. These projects will collect comprehensive data on protein structure. The e-msd has contributed to the detailed data representation model(s) and exchange data formats and mechanisms between each step in a structure determination. This model, incorporates the means for making the information reliable, accurate and up to date and to include indicators of reliability. The e-msd recognizes that in order for data to be used efficiently for searches within the database, and have ensured data uniformity in that the meta-description of the data is consistent across all entries. The e-msd not only allows for data harvesting and archival of clean cross referenced structural data, search mechanisms are being developed to allow research workers to for example automatically annotate structure motifs and binding site properties.

KEYWORDS: DATA HARVESTING DATA REPRESENTATION STRUCTURE ANNOTATION

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PERSPECTIVES IN COMPUTATIONAL MOLECULAR DYNAMICS

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Classical molecular dynamics is by now a well-established tool in the simulation of condensed phases. Its application to crystal structures is straightforward, provided that a reliable force field be available. This introductory talk will review some results obtained in the dynamic simulation of molecular crystals: low-T analysis of librations in ordered crystals, variable-T simulations of lattice expansion, including the entire state equation of the material, for crystals like acetic acid and succinic anhydride; simulation of crystal collapse at the melting temperature. In addition, results on the simulation of molecular motion in inclusion compounds will be described. Finally, some results on studies of nucleation of several small solutes (tetrolic acid, acetic acid, succinic anhydride) from carbon tetrachloride will be presented. Perspective for future work will be briefly discussed.

Keywords: MOLECULAR SIMULATION MOLECULAR DYNAMICS COMPUTATION

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HYSTERESIS IN FIRST ORDER PHASE TRANSITIONS; IS THERE A CLASH BETWEEN THE 'CLASSICAL' AND THE 'ACTUAL'?

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Classical thermodynamics requires that first order phase changes should be sharp and reversible, and yet there is much evidence, already emphasized by A. R. Ubbelohde many years ago (Brit. J. Appl. Phys. (1956), **7**, 313-321 “Crystallography and the Phase Rule?”; Quart. Revs. (1957). **11**, 246-272; “Thermal Transformations in Solids”), of premonitory effects and hysteresis in some solid-state phase changes, and of premonitory effects in melting. Among recent examples of hysteresis are Tl picrate (Botoshansky et al., Acta Cryst. (1994). B**50**, 589-596) and perylene (Botoshansky et al., in preparation (2002)). Much detail emerges from the complementary studies. of Mitkevic et al. (Acta Cryst. (1999). B**55**, 799-806), who demonstrated, by XRD, co-existence of phases in the phase changes occurring in 4,4[1]-dichlorobenzophenone around 190 K, and Schmidt et al. (J. Am. Chem. Soc. (1999). **121**, 11291-11299), who used ^{13}C and ^{15}N solid state NMR to show similar effects in 2-(2,4-dinitrobenzyl)-3-methylpyridine. A possible explanation for phase coexistence in bulk phases is the presence of domains subjected to different pressures because of interfacial and strain energy contributions to the total free energy. Hysteresis effects do not occur in the ultra-fast insulator-to-metal phase change in thin (200 nm) films of VO_2 (Cavalleri et al., (2001), Phys. Rev. Lett**. 87**, 237401(4)), presumably because of the absence of domains.

Keywords: PHASE TRANSITIONS HYSTERESIS PHASE COEXISTENCE

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PHASE CHANGES IN 'SOLID-SOLID' BIMOLECULAR REACTIONS

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A large number of synthetically useful reactions between solid reactants have been reported. These are usually referred to as solid-solid reactions but, in many cases, may be shown to proceed via sequential solid-liquid-solid phase transformations. The role of phase transitions in the course of reactions between solid reagents will be discussed.

Keywords: SOLID SOLID PHASE CHANGES EUTECTIC