enzyme. In addition, these studies can provide fundamental insights into how ligand binding regulates protein function. Such information has direct applications in the areas of drug discovery, regulation of metabolic pathways and other signal transduction processes.

880-Pos Board B649
Dynamics of Amyloid Beta-Peptide (21-30) and its Iowa Mutation under Confinement and Crowding: A Molecular Dynamics Study
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We present long time all-atom molecular dynamics simulations of the wild type (WT) and Iowa mutation of the amyloid β-protein (Aβ) fragment (21-30) under confinement and crowding. To study the effects of confinement, we model the protein and solvent system to be confined inside spherical pores of varying sizes (12-24Å) composed of both, hydrophilic and hydrophobic walls. We discuss the dynamics of folding, and mechanisms of unfolding from a preformed β-hairpin under both confinement types by varying the size of the confined pore. Simulation results show that the dynamics of the WT and Iowa Aβ(21-30) in confinement (hydrophobic and hydrophilic) exhibit considerable variations from the corresponding bulk simulations. Also, the unfolding of preformed β-hairpin structures follow different mechanisms based on the pore type and closeness to the confined wall. These differences in mechanism are also reflected in the lifetimes of the preformed β-hairpin structures. We present effects of crowded environments on the dynamics of the WT Aβ(21-30) by modeling the crowders as C70 and $C60(OH)_{20}$ spherical fullerenes in explicit solvent. Results and detailed comparisons between the two systems will be presented.

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Power-Law Trappings Cause Anomalous Diffusions of Water Molecules on Membrane Surfaces
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Cell membranes provide unique local environments for biological reactions, where diffusion of biomolecules as well as water molecules plays critical roles. In this study, molecular dynamics simulations for a system of water molecules / lipid bilayer were performed at temperatures from 250 K to 350 K to examine dynamics of water molecules around the surface of the lipid bilayer. Our analysis introduces a mean exit time approach which allows characterizing diffusive properties of water molecules around the surface of lipid bilayers. Using this method, we show that translational motions of water molecules around the surface of lipid bilayers are slower than those in bulk. Moreover, we find that trapping times of water molecules onto membrane surfaces are distributed according to power-law distributions depending on temperature and that water molecules on the membrane surfaces exhibit subdiffusions in translational as well as rotational motions. We provide evidence that not only an enhancement of the viscosity but also subdiffusions of water molecules on membrane surfaces originates from power-law trappings in translational motions on membrane surfaces.

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Photoisomerization Control Mechanisms in Protonated Schiff Bases
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We have performed *ab initio* excited-state molecular dynamics simulations of an isolated photo-excited protonated Schiff base (C_1-N_2=C_3-C_4=C_5-C_6) to search for mechanisms that control its photoisomerization outcome, such as the bond selectivity and (trans, cis) conformation. We observe that the photo-excited molecule twists around the N_2C_3 bond (~80% cases of the thermal ensemble) or the C_4C_5 bond, and relaxes back to the ground electronic state with either a trans or cis outcome. First, we show that a significant initial distortion of several selected dihedral angles can preferentially guide the excited-state dynamics towards twisting of the C_4C_5 bond. Next, we examine if the bond selectivity can be controlled by the vibrational pre-excitation of the molecule along individual normal modes. We find that pre-excitation of only one of the modes, which contains a prominent propelling motion of the C_4C_5 bond with respect to the neighboring C_3C_4 single bond, leads to twisting of the C_4C_5 bond. Normal mode decomposition of the ground state thermal ensemble shows that in starting structures in which this same mode is pre-excited by 1-2 k_BT thermal energy, the twisting of C_4C_5 occurs with a 30-50% probability. Finally, we find that the (trans, cis) outcome of the reaction can be controlled by selective pre-twisting of several dihedral angles, while keeping other degrees of freedom thermally excited. This choice was justified by the observed pre-twisting of retinal chromophore in rhodopsin, which exhibits 65% cis to trans transition. In the thermal ensemble with such pre-twisted dihedrals, we observe on the excited state potential energy surface synchronized twisting of CN_2C_3C and HN_2C_3H torsional angles surrounding the isomerizing N_2C_3 bond, which significantly increases the fraction of reactive (cis to trans) trajectories. These observations provide crucial understanding of natural photoisomerization mechanisms and their potential use in synthetic molecules.

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Dependency of Percolation Threshold of Water Cluster on Flexibility of Ice Nucleation Protein
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Ice nucleation protein is a planar hydrophilic protein buried in the outer cell membrane of ice nucleating active bacteria. This protein is said to induce a phase transition from liquid water to ice surfaced on it. However, the mechanism of the phase transition has not been clarified. We investigated characteristics of water clusters on the protein and interactions between water clusters and the protein by molecular dynamics simulations. We also focused on the percolation theory to analyze those clusters. As a result, behavior of water molecules depended on the existence of percolation clusters. The flexibility of the protein helped to form percolation clusters.

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Molecular Dynamics Study of the Effect of the Interface Structure on the Kinetics of Ice Crystal Growth
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Understanding the mechanisms of molecular spontaneous self-assembly is essential for the ability to predict structures of folded proteins and other complex biological structures. Precise control of material crystal structure and, therefore, its mechanical properties is another field where detailed knowledge of self-assembly is of principal interest.
Our current knowledge of the mechanisms and kinetics of such processes is still limited. In this work the spontaneous growth of ice (freezing) is studied by molecular dynamics simulations in the isoconfigurational ensemble at three different temperatures below the melting point. Ice is a molecular crystal where water molecules are held in place by hydrogen bonding, an interaction similar to interactions in biological systems. This similarity and relative simplicity of this system, at the same time, make it a perfect subject for uncovering details of ordering and disordering processes during self-organization of matter.
It is shown that specific structures determine local thermodynamics at a growing interface and directly influence kinetics of growth at a time scale of 1-2 ns due to fluctuations. The structural effect on the growth behaviour can be characterized in terms of relative growth propensities.
The topology of the initial interfaces is obtained using a structural order parameter and compared with the observed growth behaviour. Critical interfacial features specific to the observed growth patterns are identified in some cases. The work clearly indicates that local structure determines, to a large degree, the tendency of an interface to grow or melt.
This structural effect upon the ordering kinetics should be a universal behaviour and can be expected in more complex biologically relevant ordering processes.

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Effect of Monovalent Ion Concentration in Molecular Simulation of Electroporation
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Monovalent ion concentration gradients, regulated by ion pumps and leak channels, are critical components of many cellular functions. This dynamic balance is disturbed by the electroporative permeabilization of the cell membrane, which bypasses the normal membrane barriers to transmembrane ion flux. A better understanding of ion transport during and after electroporation will enable more efficient and more effective utilization of this method in biomedicine and biotechnology.
Molecular dynamics (MD) simulations provide a view of the behavior of ions and biomolecular structures at the molecular level. Previous MD studies