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THE MOLECULAR DYNAMICS AND EXPERIMENTAL STUDIES OF THE STRUCTURAL BEHAVIOR OF ALCOHOLDEHYDROGENASE ENZYME ON THE GRAPHITIC SORBENT SURFACES

In the present work the proteins'orientation and sorption dynamics on the matrices of various sorbents are investigated both experimentally and numerically. The computer molecular dynamics (MD) and experimental studies have been performed for the enzyme alcoholdehydrogenase with its co-factor (ADH+NAD) solvated by water on a graphitic carbon surface. The MD analysis provides mapping of the orientation adsorption of the ADH+NAD enzyme with a significant extension of the original basic model, thereby allowing the change in protein conformation observed in detail in the region of the ADH titratable amino acid residues. The detection of the characteristic conformation of key titratable aminoacids may become a necessary stage in further research and implementation of a numerical experiment, which will be carried out by varying the pH and charge values.

Next, based on the extension of the MD model implementation the mechanism of conformational changes in the whole system (ADH+NAD + water / graphitic carbon surface) is examined and the orientation aspects of the whole protein system along with the key titratable amino acids are studied in details. The numerical MD modeling implemented in this study use the AMBER-18 package with a fast module realization "pmemd.cuda" on a CPU/GPU cluster machine. The MD simulation data discussed with the experimental observations, which indicate on the atomic/molecular mechanism of the influence of pH solution on the proteins'conformation and orientation adsorption.

Section

Energy and materials science (Section 2)

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