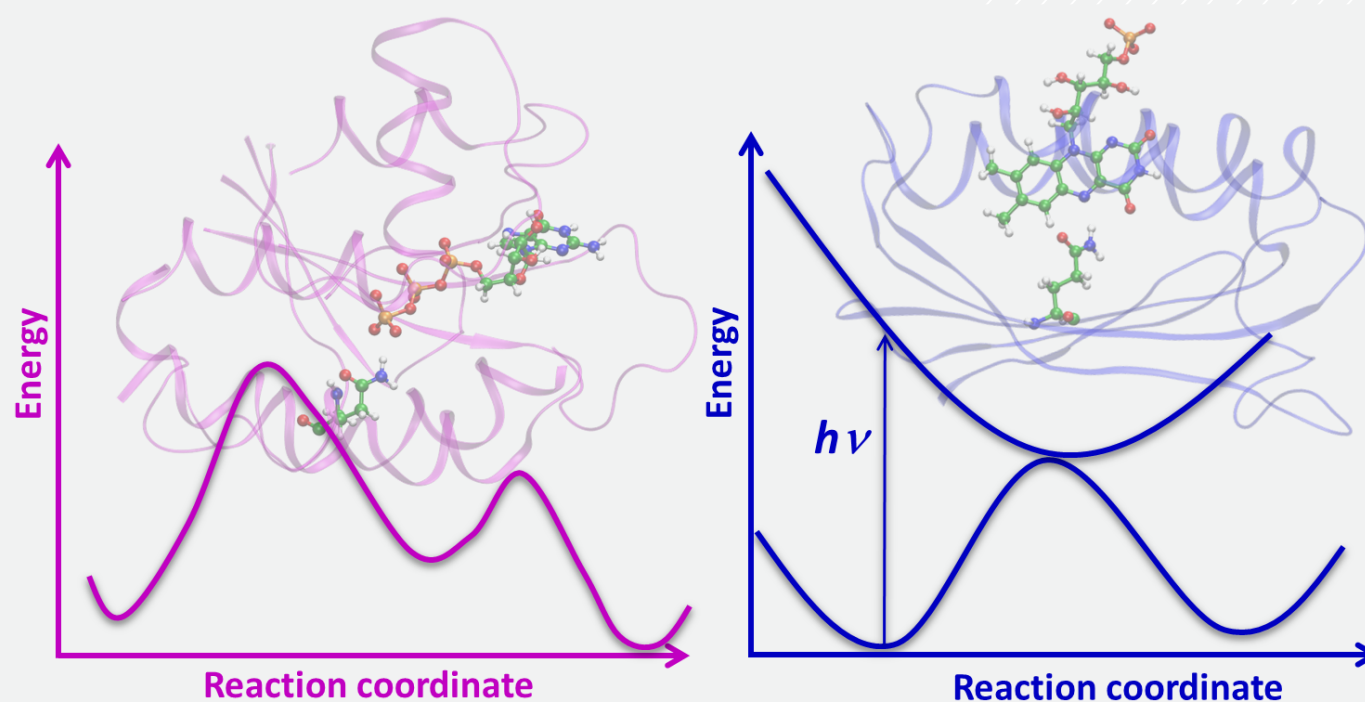


# COMPUTATIONAL MODELING OF MOLECULAR PROCESSES IN PROTEINS



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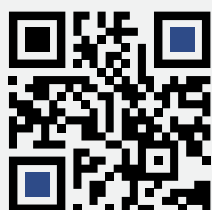


## ABSTRACT

We consider molecular processes in proteins including chemical reactions catalyzed by enzymes and photo-induced transformations in photoreceptors. Quantum mechanics/molecular mechanics (QM/MM) and molecular dynamics (MD) methods are the appropriate modeling tools for these simulations. We analyze the results of the combined QM/MM and MD simulations aiming to model kinetics in several important proteins. Simulations of the fluorescent proteins constitute another important direction of our studies using the QM/MM and MD approaches.

## BIOGRAPHY:

Alexander Nemukhin was born in Moscow in 1946, and he studied chemistry at Lomonosov Moscow State University. He got his Ph. D. in 1975 and the degree of Doctor of Sciences in 1989, both from the same University. The doctoral thesis was entitled "Multiconfigurational wavefunction expansions in the electronic structure theory". Since 1993, he is a Head of the Laboratory of Chemical Cybernetics at the Chemistry Department of Lomonosov Moscow State University. In 2006 he also took the Laboratory of Computer Modeling of Biomolecular Systems and Nanomaterials at Emanuel Institute of Biochemical Physics of Russian Academy of Sciences. In his professional career he worked as a visiting scientist at University of Minnesota, University of Wisconsin-Madison, and at the National Institute of Health (Maryland, USA).



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