

Publications list, Stefan Kolev

1. Stefan K. Kolev, Petko St. Petkov, Miroslav A. Rangelov, Georgi N. Vayssilov „Density Functional Study of Hydrogen Bond Formation Between Methanol and Organic Molecules Containing Cl, F, NH₂, OH, and COOH Functional Groups” The Journal of Physical Chemistry A, 115, 14054–14068 (2011).

In this work, I performed all quantum computational calculations, on a Linux cluster with the use of Gaussian software package. DFT hybrid functionals were employed. Geometry parameters as well as electronic structures of the complexes between methanol and organic molecules were used in order to simulate steps of the peptide biosynthesis in the ribosome.

2. Stefan K. Kolev, Petko St. Petkov, Miroslav A. Rangelov, Georgi N. Vayssilov „**Ab Initio Molecular Dynamics of Na⁺ and Mg²⁺ Counter Cations at the Backbone of RNA in Water Solution**” ACS Chemical Biology, 8 (7), 1576–1589 (2013).

In this work, I performed all quantum computational calculations, on a Bluegene P supercomputer with the use of CP2K software package. DFT quantum dynamics was employed. The interaction of the ions and the phosphate groups of RNA were studied.

3. Hristo Iglev , Stefan K. Kolev, Hubert Rossmadl, Petko St. Petkov, Georgi N. Vayssilov “**Hydrogen Atom Transfer from Water or Alcohols Activated by Presolvated Electrons**” The Journal of Physical Chemistry Letters, 6 (6), 986–992 (2015)

In this work, I performed calculations of the photoexcitation and electron transfer to the medium from an OH⁻ ion. Calculations were performed in order to study the recombination mechanism of the excited electron and the remaining OH radical. The task was accomplished combining DFT (GGA-PBE) dynamical simulations of the larger system and cluster optimizations with hybrid functional. Electronic transitions were analyzed with TDDFT.

Patents and utility models

1. Photobioreactor for industrial cultivation of microalgae (Utility model application), D. Trifonov, S. Kolev, Bulgaria 2965, 2015
2. Modular photobioreactor for cultivating microalgal inoculants (Utility model application), D. Trifonov, S. Kolev, Bulgaria 2977, 2015
3. Modular installation for manufacturing plant extracts (Utility model application), D. Trifonov, S. Kolev, Bulgaria 3009, 2015