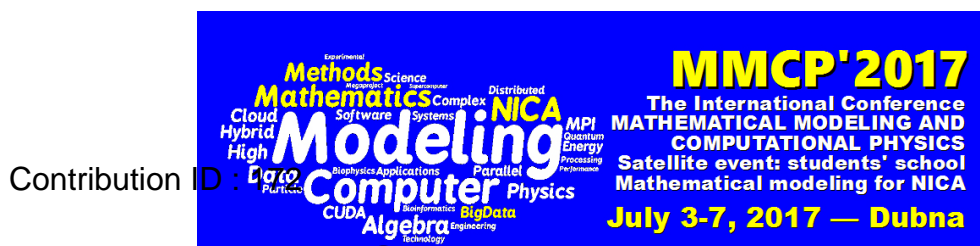


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Contribution ID :

Numerical Simulation of the Hydrated Electron States Formation

Monday 03 Jul 2017 at 17:30 (00h15')

Content :

A method and a complex of computer programs are developed for the numerical solution of the system of nonlinear partial differential equations describing a formation of the polaron states in condensed media [1,2]. Parallel implementation is based on the MPI technique and on the utilizing of the partition algorithm [3].

Numerical simulation of the photoexcited electron states formation in water under the action of the ultraviolet range laser irradiation is carried out. Our approach allows one to reproduce the experimental data on the hydrated electrons formation [2,4]. The model was modified to account for the time-dependence of the absorption band width of the hydrated electron. This modification improves an agreement of numerical results with experimental data.

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[1] V. D. Lakhno Chem. Phys. Lett. 437 P.198-202 (2007)

[2] V.D. Lakhno, A.V. Volokhova, E.V. Zemlyanaya, et al Journal of Surface Investigation: X-ray, Synchrotron and Neutron Techniques 9 (1), 7580 (2015)

[3] A.V. Volokhova, E.V. Zemlyanaya, V.S. Rikhvitskij Computational Methods and Programming (Russian) 16, 281-289 (2015)

[4] E.V. Zemlyanaya, A.V. Volokhova, V.D. Lakhno, I.V. Amirhanov, I.V. Puzynin, T.P. Puzynina, V.S. Rikhvitskiy, P.Kh. Atanasova AIP Conference Proceedings, Vol. 1684, 100006(1-9), 2015

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