Table of Contents

Contributed Papers

Ab Initio Molecular Dynamics Studies of Hydrogen Bonding and IR Spectra in EMIM-TFSI/H_2O Systems 11
P. Wróbel, P. Kubisiak, A. Eilmes

Vibrational Spectra from Molecular Dynamics: Seeking for an Efficient Computational Method 13
A. Eilmes, P. Wróbel, P. Kubisiak

Computational Modeling of Intermolecular Interactions in Supramolecular Crystals: Towards Automated Explorations of Chemical Spaces 15
G. Niedzielski, R. Podgajny, J. Hooper

Molecular Modeling of Cisplatin Derivatives: the Relationship Between Structure and Potential Bioactivity 17
W. M. Łach, M. M. Solarek, M. Nowakowska, K. Szczubiałka, M. Z. Brela

Solvent Molecules Impact on the Nylon 6 Thermal Degradation Process: the Ab Initio Molecular Dynamics and DFT Study 19
Y. Didovets, M. Z. Brela

Molecular Modeling of Selected Perovskites with Possible Application in Photovoltaics 21
A. Mikłas, M. Z. Brela

Computational Studies on Structural and Photophysical Properties of a 2,4-Dihydroxyphenyl--Substituted 1,3,4-Thiadiazole 25
D. Kaczmarczyk, A. Matwijczuk, M. Srebro-Hooper

The Strategy of a Living Organism – the Simulation Model 27
I. Roterman, L. Konieczny

Molecular Dynamics Simulations for the Michaelis Complex of Ectoine Synthase (EctC) 29
J. Andrys-Olek, J. Heider, T. Borowski

Advances in the System for the Automatic Dogs' Skin Cancer Detection 31
R. Frączek, M. Karwatowski, J. Grzeszczyk, J. Caputa, P. Pindel, D. Łukasik, M. Wielgosz, P. Russek, A. Dąbrowska-Boruch, E. Jamro, M. Pietroń, S. Koryciak, K. Wiatr

Sonochemical Formation of Fluorouracil Nanoparticles: Toward Controlled Drug Delivery from Polymeric Surfaces 33
P. Chytrosz-Wróbel, M. Gołda-Cępa, P. Kubisiak, W. Kulig, Ł. Ćwiklik, A. Kotarba

Computational Studies of Potential Mechanisms for Inhibiting the Toxicity of Amphotericin B via Molecular Association 35
M. Gurba, A. Matwijczuk, J. Hooper

Hybrid-Kinetic Simulations of Quasi-perpendicular Shocks in High Beta Cosmic Plasmas 37
S. Boula, J. Niemiec, T. Amano

Particle-In-Cell Simulation of the Leptons Acceleration in the Precursor of Young Supernova Remnant Shock 39
O. Kobzar

Differences Between Vibrational Wavepackets Generated via Singlet Fission and Those Shaped by Direct Raman Pumping 41
G. Mazur, M. Andrzejak, T. Skóra, P. Petelenz

Particle Transport Simulation for the Personalized Radiotherapy 43
L. Grzanka, S. Kania, J. Niechaj, Ł. Pitrus

Improving Hip Dysplasia Diagnosis in Dogs through Augmented 3D Video Simulation 45
K. Strzałka, S. Mazurek, M. Wielgosz, J. Caputa, R. Frączek, M. Karwatowski, J. Grzeszczyk, J. Krupiński, D. Łukasik, A. Śmiech, P. Russek, A. Dąbrowska-Boruch, E. Jamro, M. Pietroń, S. Koryciak, K. Wiatr

Development of the Machine Learning Based Track Reconstruction in the MUonE Experiment 49
M. Zdybał, M. Kucharczyk, M. Wolter

Deep Neural Networks for the Calibration of Timing Detectors 51
M. Kocot, K. Misan, V. Avati, E. Bossini, L. Grzanka, N. Minafra

Neural Networks for the Analysis of Particle Tracing in PIC Simulations 53
G. Torralba Paz, A. Bohdan, J. Niemiec

Dog Gait Assessment Using Temporal Graph Neural Networks 55
S. Mazurek, K. Strzałka, M. Wielgosz, J. Caputa, R. Frączek, M. Karwatowski, J. Grzeszczyk, J. Krupiński, D. Łukasik, A. Śmiech, P. Russek, A. Dąbrowska-Boruch, E. Jamro, M. Pietroń, S. Koryciak, K. Wiatr

Do Cohort Studies in Diffusion MRI Require a Marriage of Convenience with High-Performance Computing? A Case Study 59
D. Ciupek, J. Machnio, M. Malawski, T. Pięciak

Classification of Images of Cytological Samples for the Purposes of Initial Analysis 61
J. Krupiński, S. Mazurek, K. Strzałka, M. Wielgosz, J. Caputa, R. Frączek, M. Karwatowski, J. Grzeszczyk, D. Łukasik, A. Śmiech, P. Russek, A. Dąbrowska-Boruch, E. Jamro, M. Pietroń, S. Koryciak, K. Wiatr

Leveraging ACC Resources for Medical Research 63
P. Nowakowski, M. Bubak, K. Gądek, M. Kasztelnik, M. Malawski, J. Meizner, A. Nowak, P. Połeć, K. Zając, T. Zhyulin

Towards Observability in Scientific Computing 65
B. Baliś, A. Kuźma, Ł. Wroński

UWLCM – Eulerian-Lagrangian Cloud Model for Heterogeneous Computing Clusters 67
P. Dziekan, P. Żmijewski

Unsupervised Detection of Decoupled Subspaces in the Quantum Hilbert Space 69
T. Szołdra, P. Sierant, M. Lewenstein, J. Zakrzewski

Scalability of a Neuroevolutionary Based Framework for Anomaly Detection 71
M. Pietroń, D. Żurek, K. Faber

Author Index 73