Curriculum Vitae of Zoltán Ható

Born: 1985, Tatabánya, Hungary

Education:

High school: (1997-2003)

Árpád Secondary Grammar School, Tatabánya, Hungary

2003 Secondary grammar school maturity certificate

University: (2003-2011)

University of Pannonia, Veszprém, Hungary

2011 Master of Information Technology in Chemsitry

(Simulation study of membranetransport in flexible zeolite framework)

Supervisor: Dr. Tamás Kristóf, University of Pannonia , Department of Physical Chemistry

Ph.D student (2011-2014)

Doctoral School of Chemistry and Environmental Sciences ,University of Pannonia, Veszprém, Hungary

Supervisor: Dr. Tamás Kristóf, University of Pannonia , Department of Physical Chemistry

2014 Absolutorium (all of the academic requirements for the degree are completed, except the dissertation)

Ph.D. Candidate(2014-)

Experience

Participating in a project entitled Multipurpose radiotracer method for the investigation of contamination and corrosion phenomena on constructional material surfaces. My main tasks were calculating compositions of solutions and ascertain speciation in equilibrium and quasi-equilibrium systems with thermodynamic modelling. (employment contracts as student 2010.07.16. - 2010.12.31. and 2011.03.08.-2011.05.31.)

Participating in Mobility and Environment, Research of Automotive Industry, Energetics and Environment in the Middle- and Western-Danubian Region Nr. 1. Course, in the frames of the sub-topic called PE/1.1.8. (TÁMOP-4.2.1/B-09/1/KONV-2010-0003 tender). I mainly participated in investigation of structure and thermodynamic properties of electrorheological fluids with molecular simulations. (2012.03.01. - 2012.07.29.)

Since 2014 I am a participant in a Hungarian National Research Fund (OTKA) project entitled "Bioinspired nanomaterials" led by Dr. Dezső Boda and I am an employee of the University of Pannonia as a research worker at the Department of Physical Chemistry.

In 2015 I have got a research scholarship for one year at the University of Paderborn, Department of Thermodynamics and Energy Technology (ThEt). I worked on the computer simulation of large systems with high-performance computing resources (OCuLUS HPC Cluster with GPU Accelerators and Large Shared-Memory Nodes). We modeled the intercalation and delamination processes of kaolinite (with realistic layer size) in potassium acetate and hexylamine solutions.
Consultant: Dr. Jadran Vrabec, Dr. Tamás Kristóf

Languages and levels

hungarian (mother language)

german (CEFR B2 ,language exam: intermediate C)

english (CEFR B2)

Professional activity

My main research focus is on molecular simulation of adsorption and diffusion phenomena on multi-scale levels (spatial size and time scale). I work mostly with my colleagues at the Department of Physical Chemistry (Tamás Kristóf, Dezső Boda, Mónika Valiskó), at the Institute of Materials Engineering (Éva Makó, András Kovács) and with students at our department (Ákos Kaviczki, Richárd Katona). I also collaborate with international coworkers (Jülich, Germany :Casasnovas Perera Rodrigo, Paolo Carloni; Kaiserslautern, Germany:Martin Horsch; Paderborn, Germany: Jadran Vrabec, Gábor Rutkai, and Chicago, USA: Dirk Gillespie)

Usually I teach in fall semester the problem solving practice in physical chemistry course.

Since 2012 I am a member of Physics Subcommittee in Regional Centre of the Hungarian Academy of Sciences, Veszprém.

I am involved in the Student Research Societies (TDK). I participated as student and later I helped organize the events, I was the secretary of the Society at the Faculty of Engineering between 2012 and 2015. Since 2015, I am one of the secretaries of the Society at the University of Pannonia.). In April of 2015, we organized the National TDK Conference in the Chemistry and Chemical Industry Section in Veszprém.

Science metric data:

Total Impact Factor: 19.536

IF (2015): 3.844

Number of independent citations: 7

Number of talks at conferences: 2

Current courses and research:

My current activity involves Molecular Dynamics (MD) simulation of membrane diffusion (biological ionchannels, zeolite membranes or simple “toy model” channels) and MD simulations of kaolinite intercalation and delamination processes with different intercalated interlayer molecules. Me and my coworkers are always eager to develop new simulation methods and incorporate them into existing simulation tools (either into our homemade codes or into available free software).

Most recently in the Computer modeling research group at the Department of Physical Chemistry we are working on bipolar channels investigated by all-atom MD simulations compared to results provided by the Nernst-Planck coupled to Local Equilibrium Monte-Carlo method using a reduced model.

List of publications:

[10] Simulation study of a rectifying bipolar ion channel: Detailed model versus reduced model
Z Ható, D Boda, D Gillespie, J Vrabec, G Rutkai, T Kristóf
Condensed Matter Physics 19 (1), 13802 (2016) IF: 0.748

[9] Stability of the kaolinite-guest molecule intercalation system: A molecular simulation study
G Rutkai, Z Ható, T Kristóf
Fluid Phase Equilibria 409, 434-438 (2016) IF:2.2

[8] Simulation assisted characterization of kaolinite–methanol intercalation complexes synthesized using cost-efficient homogenization method
É Makó, A Kovács, Z Ható, T Kristóf
Applied Surface Science 357, 626-634 (2015) IF: 2.711

[7] A simple method for the simulation of steady-state diffusion through membranes: pressure-tuned, boundary driven molecular dynamics
Z Ható, Á Kaviczki, T Kristóf
Molecular Simulation, 1-10 (2015) IF: 1.133

[6] Characterization of kaolinite–ammonium acetate complexes prepared by one-step homogenization method
É Makó, A Kovács, Z Ható, B Zsirka, T Kristóf
Journal of Colloid and Interface Science 431, 125-131 (2014) IF: 3.368

[5] Communication: Molecular simulation study of kaolinite intercalation with realistic layer size
Z Ható, G Rutkai, J Vrabec, T Kristóf
The Journal of Chemical Physics 141 (9), 091102 (2014) IF: 2.952

[4] Water-mediated potassium acetate intercalation in kaolinite as revealed by molecular simulation
Z Ható, É Makó, T Kristóf
Journal of Molecular Modeling 20 (3), 1-10 (2014) IF: 1.736

[3] Simulation of steady-state diffusion: Driving force ensured by dual control volumes or local equilibrium Monte Carlo
Z Ható, D Boda, T Kristóf
The Journal of Chemical Physics 137 (5), 054109 (2012) IF: 2.952

[2] Impact assessment of chemical decontamination base-technology's preoxidation step on different steel surfaces
E Deak-Horvath, K Varga, A Szabo-Nagy, T Kristof, Z Hato, J Schunk, ...
Korrozios Figyelo 52 (4), 73-80 (2012)

[1] Molecular simulation of water removal from simple gases with zeolite NaA
É Csányi, Z Ható, T Kristóf
Journal of Molecular Modeling, 1-8 (2011) IF: 1.736

Conferences

VII. Jahrestagung der Boltzmann-Zuse-Gesellschaft, TU Kaiserslautern
Kaiserslautern, 29-30. June 2015.
Speech: Z.Ható A dæmon for steady-state diffusion through membranes

9th Liquid Matter Conference Lisbon
Lisbon, Portugal 21-25 July 2014
Poster: D Boda, D Gillespie, M Valiskó, Z Ható, T Kristóf Simulating Ion Transport through Selective and Rectifying Ion Channels Using Local Equilibrium Monte Carlo

9th Liblice Conference on the Statistical Mechanics of Liquids
Congress Hotel JEZERKA at the Sec Dam Lake, 15-20 June. 2014
Poster: Z. Ható, G. Rutkai, J. Vrabec T. Kristóf Molecular simulation study of kaolinite intercalation with realistic layer size

12th Joint European Thermodynamics Conference
Brescia, Italy 1-5 July 2013
Poster: Ható Z., Makó É., Kristóf T. Molecular simulation study of kaolinite intercalation
Poster: Ható Z., Gillespie D., Kristóf T., Boda D. Computer simulation of a rectifying ion channel

XXXV. Kémiai Előadói Napok, Szeged, 2012. október 29-31.
Speech: Stacionárius diffúzió molekuláris szimulációja Monte-Carlo módszerrel

2012 Annual Meeting of the European Molecular Liquids Group and Japanese Molecular Liquids Group, Molecular association in fluid phases and at fluid interfaces
Eger, Hungary 5-9 september 2012
Poster: Z. Ható, D. Boda, T. Kristóf, Direct simulation of steady-state diffusion by classical Monte Carlo methodologies