

CPBCI 2019
2-6 June 2019
Eger, Hungary

Chemistry, Physics and Biology of Colloids and Interfaces

2-6 June 2019, Eger, Hungary



BOOK OF ABSTRACTS

Conference Program

Sunday, 2 June

17.40-18.00: Conference opening

Session 1 (chair: Angéla Jedlovszky-Hajdú):

18.00-19.00: **Miklós Zrínyi** (Budapest, Hungary): *Neutral colloidal particles and polymers in electric field*

19.00-21.00: Welcome reception

Monday, 3 June

Session 2 (chair: István Szilágyi):

09.00-10.00: **Michal Borkovec** (Geneva, Switzerland): *Forces between Colloidal Particles in Aqueous Solutions*

10.00-10.20: **Tamás Szabó** (Szeged, Hungary): *Semiconductor nanoparticle/graphene oxide composites for environmental applications*

10.20-10.40: **Dóra Barczikai** (Budapest, Hungary): *Biocompatible fibrous meshes incorporating silver nanoparticles for wound dressing applications*

10.40-11.00: **Etelka Tombácz** (Szeged, Hungary): *On the analogies and peculiarities of charging and colloidal stability of humic acids and graphene oxides*

11.00-11.30: Coffee break

Session 3 (chair: Sofia Kantorovich):

11.30-12.30: **Francesco Sciortino** (Rome, Italy): *Gels of DNA*

12.30-12.50: **Livia Naszályi-Nagy** (Gent, Belgium): *DNA building block adsorption on SiO₂@ZrO₂ NPs*

12.50-13.10: **Rita Varga** (Budapest, Hungary): *Poly(aspartic acid) based nano gel fibers for tissue engineering*

13.10-14.30: Lunch

Session 4 (chair: Dezső Boda):

14.30-15.30: **Ilan Benjamin** (Santa Cruz, USA): *Surface-active molecules influence on charge transfer reactions at liquid interfaces*

15.30-16.00: Coffee break

16.00-18.00: POSTER SESSION

Tuesday, 4 June

Session 5 (chair: Tamás Szabó):

- 09.00-10.00: **Judit Puskas** (Akron, USA): *Folic acid conjugated polymeric nanocarrier for targeted cancer detection in hepatocellular carcinoma*
- 10.00-10.20: **Kristóf Molnár** (Budapest, Hungary): *Biocompatible, biodegradable and implantable poly(amino acid) based fibrous networks*
- 10.20-10.40: **Tímea Pernyeszi** (Pécs, Hungary): *Use of microorganisms in environmental bioremediation*
- 10.40-11.00: **Ákos Juhász** (Budapest, Hungary): *Creating electrospun 3D artificial matrices for biomedical purposes*
- 11.00-11.30: Coffee break

Session 6 (chair: Etelka Tombácz):

- 11.30-12.30: **Ladislau Vekas** (Timisoara, Romania): *Structural characterization of aqueous magnetic fluids stabilized by sodium oleate*
- 12.30-12.50: **Anatolii Nagorny** (Dubna, Russia): *Structural characterization of aqueous magnetic fluids stabilized by sodium oleate*
- 12.50-13.10: **Deniz Mostarac** (Vienna, Austria): *The impact of structural inhomogeneities, superparamagnetism and central attraction, on the equilibrium structure of magnetic filaments*
- 13.10-14.30: Lunch

Session 7 (chair: Milan Předota):

- 14.30-14.50: **Erzsébet Illés** (Szeged, Hungary): *Multifunctional PEG-carboxylate copolymer coated nanomagnets for biomedical application*
- 14.50-15.10: **Oleksandr Artykulnyi** (Dubna, Russia): *Impact of poly (ethylene glycol) concentration and molecular mass on the structure and interaction parameters of anionic surfactant micellar solutions*
- 15.10-15.30: **Michael Bley** (Freiburg, Germany): *Molecular Simulation of Thermodynamic Properties with the Osmotic Equilibrium Approach: Accessing Activities in Complex Concentrated Liquid Phases*
- 15.30-16.00: Coffee break

Session 8 (chair: George Horvai):

- 16.00-16.20: **Ondrej Kroutil** (České Budějovice, Czech Republic): *VSFG spectrum prediction from classical molecular dynamics simulations*
- 16.20-16.40: **Dezső Boda** (Veszprém, Hungary): *Ionic transport through nanopore devices: diodes, transistors, sensors*
- 16.40-17.00: **Milan Předota** (České Budějovice, Czech Republic): *Simulations of ions and oxalic acid on rutile and quartz surfaces*
- 17.00-17.20: **Réka Horváth** (Budapest, Hungary): *Investigation of methylamine at aqueous surfaces by computer simulation methods*
- 17.20-17.40: **Gargi Joshi** (Nomi, Japan): *Controlling the Oriented Deposition of LC Polysaccharide at Evaporative Interface in a Confined Geometry*
- 17.40-18.00: **Bálint Kiss** (Lille, France): *Investigation of the thermodynamic properties and the liquid-vapor interface in formamide-water systems*
- 19.00-22.00: Wine tasting (optional event)

Wednesday, 5 June

Session 9 (chair: Angéla Jedlovsky-Hajdú):

- 09.00-10.00: **Kenneth Dawson** (Dublin, Ireland): *Nanotherapies, Risk and Opportunity; Interaction of Nanoscale Objects with Living Organisms*
- 10.00-10.20: **Viktória Varga** (Szeged, Hungary): *Investigation of different human serum albumin-based composites for kynurenic acid drug delivery*
- 10.20-10.40: **Constantinos Voniatis** (Budapest, Hungary): *Poly(vinyl alcohol) as a potential material for new surgical meshes*
- 10.40-11.00: **György Hantal** (Vienna, Austria): *On molecular mechanisms of general anesthesia*
- 11.00-11.30: Coffee break

Session 10 (chair: Róbert Mészáros):

- 11.30-12.30: **Giancarlo Franzese** (Barcelona, Spain): *From Nanomaterials to Perspectives for Brain Cancer Treatments*
- 12.30-12.50: **Dávi Juriga** (Budapest, Hungary): *Poly(aspartic acid) hydrogels: potential scaffold for tissue engineering*
- 12.50-13.10: **Krisztina Tóth** (Budapest, Hungary): *Characterization of dopamine containing fibrous polymer-drug conjugates*

13.10-14.30: Lunch

Session 11 (chair: Imre Varga):

14.30-15.30: **Imre Dékány** (Szeged, Hungary): *Protein/ polyelectrolyte/ gold self-assembled structures: drug delivery and sensor applications*

15.30-16.00: Coffee break

Session 12 (chair: Oleksandr Tomchuk):

16.00-16.20: **Róbert Mészáros** (Komarno, Slovakia): *Effect of Added Surfactant on the Poly(Ethyleneimine)-Assisted Gold Nanoparticle Formation*

16.20-16.40: **Bence Fehér** (Budapest, Hungary): *Structural Investigation of Red Fluorescent Bovine Serum Albumin-Gold Complexes*

16.40-17.00: **Łukasz Lamch** (Wrocław, Poland): *NMR studies upon aggregation behavior of hydrophobically functionalized poly(4-styrenesulfonic-co-maleic acid)*

17.00-17.20: **Abdenacer Idrissi** (Lille, France): *Self-association process in urea, acetone, acetamide and choline chloride aqueous solutions: Vibartion spectroscopy and molecular dynamics simulation*

17.20-17.40: **Eszter Mádai** (Darmstadt, Germany): *Using nanopores as sensors: The effect of the charge pattern from symmetric to asymmetric leading to a dual-response device*

17.40-18.00: **Margaret Rosenberg** (Vienna, Austria): *Self-assembly of hollow colloidal silica cubes*

18.00-22.30: Conference Banquet

Thursday, 6 June

Session 13 (chair: Pál Jedlovsky):

09.00-09.30: **George Horvai** (Budapest, Hungary): *Deeper insight into the surface tension of common solvents and of the aqueous solutions of common surfactants*

09.30-10.00: **Sofia Kantorovich** (Vienna, Austria): *In-silico study of randomly crosslinked nanogel*

10.00-10.20: **Balázs Fábián** (Prague, Czech Republic): *Investigation of the dynamics of fluid interfaces*

10.20-10.40: **Andrew Milne** (Glasgow, UK): *Polarisation Corrections and the Hydration Free Energy of Water*

10.40-11.00: **Martin Kaiser** (Vienna, Austria): *Self-propelled Dipolar Nanocubes*

11.00-11.30: Coffee break

Session 14 (chair: Abdenacer Idrissi):

11.30-12.00: **István Szilágyi** (Szeged, Hungary): *Co-immobilization of superoxide dismutase and horseradish peroxidase on polyelectrolyte-functionalized layered double hydroxide particles*

12.00-12.30: **Oleksandr Tomchuk** (Dubna, Russia): *Fractal aggregation in tetraethoxysilane/ethanol/water solutions by SANS*

12.30-12.50: **Imre Varga** (Budapest, Hungary): *A novel method for surfactant binding isotherm measurements of polyelectrolyte/surfactant mixtures validated by neutron scattering data*

12.50-13.10: **Ildikó Tóth** (Szeged, Hungary): *Wetting and properties of carbon nanotube buckypapers doped by hydrophilic nanowires*

13.10-13.20 Conference closing

13.20-14.30: Lunch

List of Posters

1. **Krisztina Bali** (Budapest, Hungary): *Oppositely charged polyelectrolyte/surfactant assemblies as emulsion stabilizing agents*
2. **Zuzana Benková, Peter Čakánek** (Bratislava, Slovakia): *Interactions of peptides with poly(ethylene oxide) grafted onto carbon nanotubes*
3. **Denys Biryukov** (České Budějovice, Czech Republic): *A General Tool for Zeta Potential Predictions from Molecular Simulations*
4. **Dezső Boda** (Veszprém, Hungary): *A scaling behavior of the transport of multivalent ions through rectifying nanopores*
5. **Joanna Feder-Kubis** (Wrocław, Poland): *Ionic liquids with natural terpene derivative as an effective fungicidal and protective preparation for the preservation of historical paper*
6. **Máté Gulácsi** (Budapest, Hungary): *Optical properties of hydrogel fiber membranes*
7. **György Hantal** (Vienna, Austria): *Chemistry and water dynamics at the surface of hydrated magnetite*
8. **Anna Harsányi** (Budapest, Hungary): *Preparation of Poly(N-isopropylacrylamide-co-4-vinylimidazole) microgel particles*
9. **Zoltán Ható** (Veszprém, Hungary): *Molecular simulation of kaolinite layer curling*
10. **Kevin Herman** (Szeged, Hungary): *Heterocoagulation assisted synthesis of zirconia/graphite oxide nanocomposites*
11. **George Horvai** (Budapest, Hungary): *Selective adsorption of basic compounds from aprotic solvents onto acidic polymers*
12. **Erzsébet Illés** (Szeged, Hungary): *Tuneable magnetic hyperthermia properties of pristine and mildly reduced GO/MNP nanocomposites*
13. **Attila Kardos** (Budapest, Hungary): *Synthesis of chemically modifiable p(HEMA)-b-PEG block copolymer*
14. **Łukasz Lamch** (Wrocław, Poland): *Synthesis and biological properties of new mild amidebetaine and amidesulfohydroxybetaine-type amphoteric surfactants*
15. **Lydie Plačková** (České Budějovice, Czech Republic): *Dynamic properties of aqueous solutions of atomic and molecular ions – effect of scaled charges*
16. **Csaba Róth** (Budapest, Hungary): *Preparation of multilayer “smart” nanocapsules*
17. **Evelin Sipos** (Budapest, Hungary): *Damage formation in weak planar fiber texture*
18. **Ildikó Tóth** (Szeged, Hungary): *Wettability characterization of carbon cloth type gas diffusion layer via infrared thermography and contact angle analysis*
19. **Mónika Valiskó** (Veszprém, Hungary): *Modeling of pH tunable nanodevices*
20. **Tamás Veres** (Budapest, Hungary): *Electrospun magnetic scaffold for theranostics*

Ionic transport through nanopore devices: diodes, transistors, sensors

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ABSTRACT

Computer simulation results for ionic transport through synthetic nanopores is presented. Nanopores serve as the core units of various nanodevices such as diodes [1,2], transistors [3], and sensors [4,5]. We study how the output signals given by the devices as responses to input signals (device functions) depend on the properties of nanopores. The device functions are rectification, switching, selectivity, and sensitivity of sensing. Also, we study these systems in a multiscale approach using models of various resolutions computed by the suitable simulation methods. We are interested in the question of what molecular details need to be included in the model in order to reproduce the device behavior. We investigate the applicability of reduced models and study what degrees of freedom should be included in the model and what degrees of freedom can be omitted. We show results of molecular dynamics (MD) simulations for all-atom models, Monte Carlo simulations for reduced models, and a mean-field continuum theory (Poisson-Nernst-Planck) for point ions. The parameters of the reduced models can be fitted either to MD data or experimental data. We will show examples for both.

REFERENCES

- [1] Ható, Z.; Valiskó, M.; Kristóf, T.; Gillespie, D.; Boda, D., "Multiscale modeling of a rectifying bipolar nanopore: explicit-water versus implicit-water simulations", *Phys. Chem. Chem. Phys.*, **19**, 17816 (2017).
- [2] Valiskó, M.; Matejczyk, B.; Ható, Z.; Kristóf, T.; Má dai, E.; Fertig, D.; Gillespie, D.; Boda, D., "Multiscale analysis of the effect of surface charge pattern on a nanopore's rectification and selectivity properties: from all-atom model to Poisson-Nernst-Planck", *J. Chem. Phys.*, in press (2019).
- [3] Má dai, E.; Matejczyk, B.; Dallos, A.; Valiskó, M.; Boda, D., "Controlling ion transport through nanopores: modeling transistor behavior", *Phys. Chem. Chem. Phys.*, **20**, 24156 (2018).
- [4] Má dai, E.; Valiskó, M.; Dallos, A.; Boda, D., "Simulation of a model nanopore sensor: ion competition underlies device behavior", *J. Chem. Phys.*, **147**, 244702 (2017).
- [5] Má dai, E.; Valiskó, M.; Boda, D., "The effect of the charge pattern on the applicability of a nanopore as a sensor", *J. Mol. Liq.*, in press (2019).

Using nanopores as sensors: The effect of the charge pattern from symmetric to asymmetric leading to a dual-response device

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ABSTRACT

Artificial nanopores the basic elements of nanofluidic devices. These devices can be used as parts of nanofluidic circuits, or for filtering and sensing thank to the rapid improvement in experimental techniques. Chemical modifications on the nanopores' wall make it possible to bind certain ions selectively, thus the nanopore can function as a sensor. In this work, a systematic modeling study about the application of a nanosensor is made via optimizing the charge pattern on the nanopore's wall in order to improve the efficiency of the sensor.

As an effect of an applied electric field, ions move through the pore. Ions of the background electrolyte serve as the main charge carriers. The binding sites (modeled with a square-well potential) selectively bind the analyte ions. This binding, on the other hand, influences the current of the background electrolyte. We analyze various mechanisms of sensing based either on the competition of the background cation with the analyte cation for space in a negatively charged nanopore region [1] or on attraction between the analyte cation and the background anion in a positively charged region [2]. Which mechanism takes action depends on the charge pattern. We show that the latter mechanism makes it possible to detect analyte ions in trace concentrations. We also show that using a nanopore with an asymmetric charge pattern makes it possible to construct a dual response device: both current and rectification serve as signals sensitive to the presence of analyte ions.

In this work, the Nernst-Planck transport equation is used to compute current together with the Local Equilibrium Monte Carlo method that is suitable to simulate ions in trace concentrations due its grand canonical design. Electrolyte is modeled as hard-sphere ions in an implicit-water background.

REFERENCES

- [1] E. Má dai, M. Valiskó, A. Dallos, D. Boda, "Simulation of a model nanopore sensor: ion competition underlies device behavior", *J. Chem. Phys.* **147**(24):244702, (2017).
- [2] E. Má dai, M. Valiskó, D. Boda. "The effect of the charge pattern on the applicability of a nanopore as a sensor", *J. Mol. Liq.* in press (2019).

Modeling of pH tunable nanodevices

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ABSTRACT

The pH of an electrolyte is an experimentally controllable parameter: pH affects the ratio of the protonated/deprotonated forms of the functional groups anchored to the inner surface of the nanopore. Change in the surface charge, in turn, changes the conductance properties of the pore that makes it possible to use nanopores as sensors [1], diodes, or transistors [2,3]. We relate the surface charge to pH and perform particle simulations (Local Equilibrium Monte Carlo [4]) to compute the ionic flux. Here we present results for two model nanodevices: transistors and sensor. In the case of a *transistor* the current is considerable in the “acidic” and “basic” regions, because the pore contains *either* positive *or* negative surface charges, so *either* anions *or* cations carry current. Current is very small in the “neutral” region, because the pore contains *both* negative *and* positive surface charges, so *both* cations *and* anions have depletion zones. This switch like behavior is controlled by the pH-dependent surface charge pattern. The behavior of our pH-responsive models is characteristically different in the different pH regions. *Nanosensors* selectively bind the analyte ions with which the ionic current flowing through the pore is changed because the local concentrations of the ions of the background electrolyte changes. The analyte concentration can be determined from calibration curves. Inspired by experimental works in the field of nanosensing we constructed asymmetric nanopores with various charge patterns to mimic the pH tunable behavior. The geometrical asymmetry produces an additional device function, rectification, resulting in a dual responsive device. The mechanism behind pH-control of ionic current can be explained by formation of depletion and accumulation zones.

REFERENCES

- [1] Má dai, E.; Valiskó, M.; Boda, D., “The effect of the charge pattern on the applicability of a nanopore as a sensor”, J. Mol. Liq., in press (2019).
- [2] Má dai, E.; Matejczyk, B.; Dallos, A.; Valiskó, M.; Boda, D., “Controlling ion transport through nanopores: modeling transistor behavior”, *Phys. Chem. Chem. Phys.*, **20**, 24156 (2018).
- [3] Fertig, D.; Valiskó, M.; Boda, D., “Controlling ionic current through a nanopore by tuning pH: a Local Equilibrium Monte Carlo study”, *Mol. Phys.*, in press (2019).
- [4] Boda, D.; Gillespie, D., “Steady state electrodiffusion from the Nernst-Planck equation coupled to Local Equilibrium Monte Carlo simulations”, J. Chem. Theory Comp., **8**, 824 (2012).