Anexa nr. 5 *Curriculum Vitae*

ROMÂNIA
MINISTERUL APĂRĂRII NAŢIONALE
ACADEMIA NAVALĂ "MIRCEA CEL BĂTRÂN"
Anexa la Cererea nr. din

CURRICULUM VITAE (model EUROPASS)

INFORMAŢII PERSONALE

Vatamanu Petrisor Jenel

Constanta, Romania

Phone: +40 792 097 290

email: jenel.vatamanu@anmb.ro

https://orcid.org/0000-0003-0825-1608

Sexul: Male

Data nașterii: 27/02/1970

Naționalitatea: Romania

LOCUL DE MUNCA PENTRU CARE SE CANDIDEAZĂ
POZIŢIA
LOCUL DE MUNCĂ DORIT
STUDIILE PENTRU CARE SE CANDIDEAZĂ
PROFILUL PERSONAL

CERCETATOR STIINTIFIC II - CIVIL,
CHIMIE ,
poziția 6 (ID 1530606).
ANMB

EXPERIENŢA PROFESIONALĂ

POZITIA CURENTA

Cercetător Științific 3 in Chimie la Academia Navala „Mircea cel Batran”, Constanta, Romania
www.anmb.ro

2016-2022

Participant ca full-time „Senior-Fellow” la ARL-RAP via ORAU, Maryland, USA
Departamentul de Electrochimie (former „Battery”)

2011-2016

Research Associate
University of Utah, Depatrment of Material Sciences and Engineering, USA
www.utah.edu

2008-2011

Postdoctoral Researcher
University of Utah, Depatrment of Material Sciences and Engineering, USA
www.utah.edu

2006-2008

Postdoctoral Researcher

University of Missouri Columbia, Department of Chemistry, MO, USA

https://missouri.edu/

2004-2006

Postdoctoral Fellow at the Dalhousie University, Halifax, NS, Canada (www.dal.ca) (between 2004-2005) and University of Calgary, Chemistry Department, AB, Canada (www.ucalgary.ca) (netween 2—5-2006) – I worked on tthe same project(s) and with the same Faculty Advisor.

EDUCAŢIE ŞI FORMARE

1999-2004

Ph. D. (doctorat)
Domeniul: Chimie Teoretica si Computațională
Queen's University, Chemistry Department, Kingston, Ontario, Canada
www.chem.queensu.ca

1995-1996

Master

Domeniu: Chimie Fizica

Alexandru Ioan Cuza University, Iași, Romania, Facultatea de Chimie

www.uaic.ro

1989-1995

Licența in Chimie

Domeniul: secția Chimie-Fizica.

Universitatea „Dunărea de Jos", Galați, Romania, Facultatea de Litere si Științe

www.ugal.ro

COMPETENTE PERSONALE

Limba maternă: Romana

Limbi străine: Engleza (fluent)

COMPETENTE DE DOMENIU DE ACTIVITATE

CHIMIE TEORETICA SI COMPUTATIONALA

Appendix

Alte informatii atasate: Mai jos este CV-ul in engleza si in format normal:

Dr. Jenel Vatamanu

Scientist
"Mircea cel Batran" Naval Academy, Str. Fulgerului, Nr. 1, Constanta, Romania, 900218
Email: jenel.vatamanu@anmb.ro
Phone: +40 727 987 416
Orcid: 0000-0003-0825-1608

Background

Over the years, I studied a large variety of physical phenomena such as the nucleation and growth of crystals, the electrode-electrolyte electrified interface, and the energy storage mechanisms in electricity-based storage devices. I have extensive experience with atomistic simulations of condensed phases, development of classical molecular dynamics (MD) methodologies and their implementation in computer codes. I am author and co-author of multiple articles published in premier journals such as *Journal of Chemical Theory and Computations, PNAS, ACS Nano, Energy Storage Materials, ACS Energy Letters, Advanced Energy Materials, Nature Communications, Nature Nanotechnology, Energy & Environmental Science*, and *Joule*. My recent studies address research topics of great interest today, such as safe and non-polluting energy storage by electrochemical batteries and supercapacitors, marine environment pollution, microplastics, shockwaves, detonations, explosions.

Current research interest:

Energy storage, renewable energy, inclusion compounds for energy storage, supercapacitors, electrochemical batteries, hydrogen storage, asphaltenes, solid-state electrolytes for energy storage systems, gas hydrates, hydrogen storage in clathrate inclusion compounds, crystallization, atomistic and molecular modelling, computer code development/maintenance, marine environment and pollution, microplastics, detonation and explosions, shockwaves.

Education:

- **Ph. D.**, Theoretical and Computational Chemistry, Queen's University, Kingston, ON, Canada, 2004
- **M. Sc.**, Physical Chemistry, Al. I. Cuza University, Iasi, Romania, 1996.
- **B. Sc.**, Physical Chemistry, Dunarea de Jos University, Galati, Romania, 1995.

Work history, Program Participations, and Fellowships:

- **Scientist,** "Mircea cel Batran" Naval Academy, Romania, - current employment.
- **Senior Oak Ridge Associated Universities Research Fellow**, Participant as a full-time Senior Fellow to the Army Research Laboratory Research Associateship Program, (ARL-RAP) via ORAU, Open Campus, U.S. Army Research Laboratory, USA, 2016-2022
- **Research Associate**, University of Utah, Department of Material Sciences and Engineering, USA, 2011-2016
- **Postdoctoral Researcher,** University of Utah, Department of Material Sciences and Engineering, USA, 2008 – 2011
- **Postdoctoral Research Associate**, University of Missouri Columbia, Chemistry Department, USA, 2006-2008
- **Postdoc Fellow**, Dalhousie University, NS, and University of Calgary, AB, Canada, 2004-2006
- **Teaching and Research Assistant,** Al. I Cuza University, Iasi, Romania, 1996-1999

Teaching experience:

- Course of General Chemistry to the 1st year undergraduate students at "Mircea cel Batran" Naval Academy (current employment).
- Teaching Assistant to undergraduate General Chemistry laboratory (during the Ph.D. program)
- Teaching Assistant to undergraduate Physical Chemistry laboratory (during the Ph.D. program)

- Teaching Assistant to undergraduate Physical and Quantum Chemistry tutorials (during the Ph.D. program)
- Teaching Assistant to undergraduate students (during the work at Al I Cuza University)

Areas of research experience:

- Energy storage
- Renewable energy
- Electrochemical batteries
- Supercapacitors
- crystallization
- Atomistic simulations
- Fundamental research of the electric double layer structure and the dynamics of its formation
- Protective/passivating layer (SEI) formation in electrochemical batteries
- High voltage Li/Zn/Mn -ion-batteries
- Reversible energy storage in Zn-based batteries
- Conductive porous materials for efficient energy storage
- Electricity based energy storage devices: electric double layer supercapacitors. Methods to improve the non-Faradaic energy densities in supercapacitors
- Room temperature ionic liquids
- Ab-initio computations with legacy codes such as VASP and Gaussian
- Force field fitting for polarizable and non-polarizable models
- Polarizable classical force-fields for atomistic simulations
- Coarse graining and force-matching
- Code development of Molecular Dynamics (MD) simulations and Monte Carlo (MC) simulations in FORTRAN 03/08 and C/C++. Efficient parallelization of MD codes
  Computer code development in legacy MD engines such as lammps and tinker-hp
  Code/script development in python.
- Analytical theories for condensed phases (such as integral equation theories)
- Nucleation of ordered phases from disordered phases: homogeneous nucleation of crystals from liquid phases.

- Heterogeneous crystal growth
- Inclusion compounds such as gas hydrates. The mechanism of gas hydrates crystal formation from water and small hydrophobic molecules

Publications:

1) Ma Z//, Xie Z//, Liu J, **Vatamanu J***, Xing L*, Li W, "Distinct roles: Co-solvent and additive synergy for expansive electrochemical range and low-temperature aqueous batteries", *Energy Storage Materials*, **2024**, 66, 103203,
DOI: https://doi.org/10.1016/j.ensm.2024.103203

2) Yang C, Xia J, Cui C, Pollard T, **Vatamanu J**, Faraone A, Dura JA, Tyagi M, Kattan A, Thimsen E, Xu J, Song W, Hu E, Ji X, Hou S, Zhang X, Ding MS, Hwang S, Su D, Ren Y, Yang X-Q, Wang H, Borodin O*, Wang C*, "All-temperature zinc batteries with high-entropy aqueous electrolyte", *Nature Sustainability*, **2023**, 6, 325–335,
DOI https://doi.org/10.1038/s41893-022-01028-x

3) Ma L//*, **Vatamanu J**//, Hahn NT, Pollard T, Borodin O*, Petkov V., Schroeder MA, Ren Y, Ding MS, Lou C*, Allen JL, Wang C, Xu K* "Highly reversible Zn metal anode enabled by sustainable hydroxyl chemistry", *Proceedings of the National Academy of Sciences (PNAS)*, **2022**, 119, e2121138119,
DOI: https://doi.org/10.1073/pnas.2121138119

4) Luo X, Xing L*, **Vatamanu J**, Chen J, Chen J, Liu M, Wang C, Xu K, Li W "Inhibiting manganese (II) from catalyzing electrolyte decomposition in lithium-ion batteries", *Journal of Energy Chemistry*, **2022**, 65, 1,
DOI: https://doi.org/10.1016/j.jechem.2021.05.022

5) Ma Z//, Chen J//, **Vatamanu J**, Borodin O, Bedrov D, Zhou X, Zhang W, Li W, Xu K*, Xing L* "Expanding the low-temperature and high-voltage limits of aqueous lithium-ion battery", *Energy Storage Materials*, **2022**, 45, 803,
DOI: https://doi.org/10.1016/j.ensm.2021.12.045

6) Cao L//, Li D//, Pollard T//, Deng T, Zhang B, Yang C, Chen L, **Vatamanu J**, Hu E, Hourwitz MJ, Ma L, Ding M, Li Q, Hou S, Gaskell H, Fourkas JT, Yang X-Q, Xu K*, Borodin O*, Wang C* "Fluorinated interphase enables reversible aqueous zinc battery chemistries", *Nature Nanotechnology*, **2021**, 16, 902,
DOI: https://doi.org/10.1038/s41565-021-00905-4

7) Liu M, **Vatamanu J**, Chen X, Xing L*, Xu K*, Li W "Hydrolysis of LiPF6-Containing Electrolyte at High Voltage", *ACS Energy Lett.* **2021**, 6, 2096, DOI: https://doi.org/10.1021/acsenergylett.1c00707

8) Chen L, Zhang J, Li Q, **Vatamanu J**, Ji X, Pollard TP, Cui C, Hou S, Chen J, Yang C, Ma L, Din MS, Garaga M, Greenbaum S, Lee H-S, Borodin O*, Xu K*, Wang C* "A 63 m Superconcentrated Aqueous Electrolyte for High-Energy Li-Ion Batteries", *ACS Energy Lett.* **2020**, 5, 968, DOI: https://doi.org/10.1021/acsenergylett.0c00348

9) Chen J, **Vatamanu J**, Xing L*, Borodin O, Chen H, Guan X, Liu X, Xu K*, Li W "Improving Electrochemical Stability and Low-Temperature Performance with Water/Acetonitrile Hybrid Electrolytes", *Advanced Energy Materials*, **2020**, 10, 1902654, DOI**:** https://doi.org/10.1002/aenm.201902654

10) Wang C, Xing L*, **Vatamanu J**, Chen Z, Lan G, Li W, Xu K* "Overlooked electrolyte destabilization by manganese (II) in lithium-ion batteries", *Nature Communications*, **2019**, 10, 3423, DOI: https://doi.org/10.1038/s41467-019-11439-8

11) Raberg JH, **Vatamanu J**, Harris S, van Oversteeg CHM, Ramos A, Borodin O, Cuk T* "Probing Electric Double Layer Composition via in-Situ Vibrational Spectroscopy and Molecular Simulations", *The journal of physical chemistry letters*, **2019**, 10, 3381-3389, DOI: https://doi.org/10.1021/acs.jpclett.9b00879

12) Dong D, **Vatamanu** J, Wei X, Bedrov D "The 1-ethyl-3-methylimidazolium bis (trifluoro-methylsulfonyl)-imide ionic liquid nanodroplets on solid surfaces and in electric field: A molecular dynamics simulation study", *The Journal of chemical physics*, **2018**, 148, 193833, DOI: https://doi.org/10.1063/1.5016309

13) **Vatamanu J***, Borodin P, Bedrov D "Application of Screening Functions as Cutoff-Based Alternatives to Ewald Summation in Molecular Dynamics Simulations Using Polarizable Force Fields", *Journal of chemical theory and computation*, **2018**, 14, 768-783, DOI: https://doi.org/10.1021/acs.jctc.7b01043

14) Wang F, Borodin O, Ding MS, Gobet M, **Vatamanu J**, Fan X, Gao T, Eidson N, Liang Y, Sun W, Greenbaum S, Xu K*, Wang C* "Hybrid Aqueous/Non-aqueous Electrolyte for Safe and High-Energy Li-Ion Batteries", *Joule*, **2018**, 5, 814-815, DOI: https://doi.org/10.1016/j.joule.2018.02.011

15) Steinruck HG, Cao C, Tsao Y, Takacs CJ, Konovalov O, Vatamanu J, Borodin O, Toney MF, "The nanoscale structure of the electrolyte–metal oxide interface", *Energy & Environmental Science*, **2018**, 11, 594-602,
DOI: https://doi.org/10.1039/C7EE02724A

16) Borodin O*, Ren R, **Vatamanu J**, von Wald Cresce A, Knap A, Xu K "Modeling Insight into Battery Electrolyte Electrochemical Stability and Interfacial Structure", *Accounts of Chemical Research*, **2017**, 50, 2886-2894,
DOI: https://doi.org/10.1021/acs.accounts.7b00486

17) **Vatamanu J**, Borodin O* "Ramifications of Water-in-Salt Interfacial Structure at Charged Electrodes for Electrolyte Electrochemical Stability", *Journal of Physical Chemistry Letter,* **2017**, 8, 4362-4367,
DOI: https://doi.org/10.1021/acs.jpclett.7b01879

18) Yang C, Chen J, Qing T, Fan X, Sun W, von Cresce A, Ding MS, Borodin O, **Vatamanu J**, Schroeder MA, Eidson N, Wang C*, Xu K* "4.0 V Aqueous Li-Ion Batteries", *Joule*, **2017**, 122-132,
DOI: http://dx.doi.org/10.1016/j.joule.2017.08.009

19) **Vatamanu J***, Borodin O, Olguin M, Yushin G, Bedrov D* (perspective, invited) Charge storage at the nanoscale: understanding the trends from the molecular scale perspective, *Journal of Materials Chemistry A*, **2017**, 40, 21049, DOI:
https://doi.org/10.1039/C7TA05153K

20) **Vatamanu J**, Bedrov D*, Borodin O "On the application of constant electrode potential simulation techniques in atomistic modeling of electric double layers", *J. Mol. Sim.*, **2017,** 43, 838-849,
DOI: https://doi.org/10.1080/08927022.2017.1279287

21) **Vatamanu J***, Bedrov D*, Vatamanu M, Borodin O "A Comparative Study of Room Temperature Ionic Liquids and Their Organic Solvent Mixtures Near Charged Electrodes", *Journal of Physics: Condensed Matter – IOPscience*, **2016,** 28, 464002-18, DOI:
https://www.doi.org/%2010.1088/0953-8984/28/46/464002

22) He Y, Qiao R*, **Vatamanu J**, Borodin O, Bedrov D, Huang J, Sumpter B "The Importance of Ion Packing on the Dynamics of Ionic Liquids during Micropore Charging" , *Journal of Physical Chemistry Letter*, **2016**, 7, 36-42,
DOI: https://doi.org/10.1021/acs.jpclett.5b02378

23) **Vatamanu J**, Ni X, Liu F, Bedrov D "Tailoring carbon-based electrodes from semiconducting to metallic for increasing the energy density in supercapacitors.", *Nanotechnology-IOP Science*, (invited, special issue), **2015**, 26, 464001-12, DOI: https://www.doi.org/10.1088/0957-4484/26/46/464001

24) **Vatamanu J***, Bedrov D "Capacitive Energy Storage: Current and Future Challenges", (perspective, invited), *Journal of Physical Chemistry Letter*, **2015,** 18, 3594-3609, DOI: https://doi.org/10.1021/acs.jpclett.5b01199

25) **Vatamanu J***, Vatamanu M, Bedrov D* "Non-Faradic energy storage by ionic liquids in nanoporous electrodes.", *ACS Nano*, **2015**, 9, 5999–6017, DOI: https://doi.org/10.1021/acsnano.5b00945

26) Bedrov D*, **Vatamanu J**, Hu Z "Ionic liquids at charged surfaces: Insight from molecular simulations", *Journal of Non-Crystalline Solids*, (special issue) **2015,** 407, 339–348, DOI: https://doi.org/10.1016/j.jnoncrysol.2014.08.007

27) Hu Z, **Vatamanu J***, Borodin O, Bedrov D "A comparative study of alkylimidazolium room temperature ionic liquids with FSI and TFSI anions near charged electrodes", **2014**, *Electrochimica Acta*, 145, 40-52, DOI: https://doi.org/10.1016/j.electacta.2014.08.072

28) Xing L*, Tu W, **Vatamanu J**, Liu Q, Huang Q, Wang Y, Zhou H, Zeng R, Li W* "On anodic stability and decomposition mechanism of sulfolane in high-voltage lithium ion battery", **2014**, *Electrochimica Acta*, 133, 117–122. DOI: https://doi.org/10.1016/j.electacta.2014.03.190

29) **Vatamanu J***, Xing L, Li W, Bedrov D "Influence of temperature on the differential capacitance of ionic liquid electrolytes on charged surfaces", **2014**, *Phys. Chem. Chem. Phys.*, *16*, 5174-5182, DOI: https://doi.org/10.1039/C3CP54705A

30) McOwen DW, Seo DM, Borodin O, **Vatamanu J**, Boyle PD, Henderson WA* "Concentrated Electrolytes: Tailoring Electrolyte Properties by Eliminating Bulk Solvent", *Energy & Environmental Science*, **2014**, 7, 416-426, DOI: https://doi.org/10.1039/C3EE42351D

31) **Vatamanu J**, Hu Z, Bedrov D*, Perez C, Gogotsi Y "Increasing Energy Storage in Electrochemical Capacitors with Ionic Liquid Electrolytes and Nanostructured Carbon Electrodes", **2013,** *Journal of Physical Chemistry Letters*, 4, 2829-2837, DOI: https://doi.org/10.1021/jz401472c

32) Hu, Z., **Vatamanu J***, Borodin O, Bedrov D "A molecular dynamics simulation study of the electric double layer and capacitance of [BMIM][PF6] and [BMIM][BF4] room temperature ionic liquids near charged surfaces"**,** *Physical Chemistry Chemical Physics*, **2013,** 15, 14234-14247,
DOI: https://doi.org/10.1039/C3CP51218E

33) Xing L, **Vatamanu J***, Borodin O, Bedrov D* "On the Atomistic Nature of Capacitance Enhancement Generated by Ionic Liquid Electrolyte Confined in Subnanometer Pores", *Journal of Physical Chemistry Letters*, **2013**, *4*, 132-140, DOI: https://doi.org/10.1021/jz301782f

34) Xing L, **Vatamanu J***, Borodin O, Smith GD, Bedrov D "Electrode/Electrolyte Interface in Sulfolane-based Electrolytes for Li-Ion Batteries: A Molecular Dynamics Simulation Study." *Journal of Physical Chemistry C*, **2012**, 116, 23871–23881, DOI: https://doi.org/10.1021/jp3054179

35) Xing L, **Vatamanu J***, Smith GD, Bedrov D "Nanopatterning of Electrode Surfaces as a Potential Route to Improve the Energy Density of Electric Double Layer Capacitors: Insight from Molecular Simulations." *Journal of Physical Chemistry Letters*, **2012**, *3*, 1124–1129, DOI: https://doi.org/10.1021/jz300253p

36) **Vatamanu J***, Borodin O, Bedrov D, Smith GD "Molecular Dynamics Simulation Study of the Interfacial Structure and Differential Capacitance of Alkylimidazolium Bis(trifluoromethanesulfonyl)imide [Cnmim][TFSI] Ionic Liquids at Graphite Electrodes", *J. Phys. Chem. C*, **2012**, 116 , 7940–7951,
DOI: https://doi.org/10.1021/jp301399b

37) **Vatamanu J***, Borodin O, Smith GD "Molecular dynamics simulation studies of the structure of a mixed carbonate/LiPF6 electrolyte near graphite surface as a function of electrode potential", *Journal of Physical Chemistry C*, **2012**, 116, 1114-1121, DOI: https://doi.org/10.1021/jp2101539

38) **Vatamanu J***, Cao, L, Borodin O, Bedrov D, Smith GD "On the influence of surface topography on the electric double layer structure and differential capacitance of graphite/ionic liquid interfaces", *Journal of Physical Chemistry Letters*, **2011**, 2, 2267-2272, DOI: https://doi.org/10.1021/jz200879a

39) **Vatamanu J***, Borodin O, Smith GD "Molecular simulations of the electric double layer structure, differential capacitance, and charging kinetics for N-methyl-N-propylpyrrolidinium

bis-(fluorosulfonyl)-imide at graphite electrodes", *Journal of Physical Chemistry B*, **2011**, 115, 3073-3084, DOI: https://doi.org/10.1021/jp2001207

40) **Vatamanu J**, Kusalik PG* "Observation of two-step nucleation in methane hydrates", *Phys. Chem. Chem. Phys.*, **2010**, 12, 15065- 15072, DOI: https://doi.org/10.1039/C0CP00551G

41) **Vatamanu J**, Borodin O*, Smith GD "Molecular insights into the potential and temperature dependences of the differential capacitance of a room-temperature ionic liquid at graphite electrodes", *Journal of the American Chemical Society*, **2010**, 132, 14825-14833, DOI: https://doi.org/10.1021/ja104273r

42) **Vatamanu J**, Borodin O, Smith GD* "Molecular dynamics simulations of atomically flat and nanoporous electrodes with a molten salt electrolyte", *Phys. Chem. Chem. Phys*, **2010**, 12, 170-182, DOI: https://www.doi.org/10.1039/B917592J

43) **Vatamanu J**, Kusalik PG, "Heterogeneous Crystal Growth of Methane Hydrate on Its sII [001] Crystallographic Face", *J. Phys. Chem. B* **2008**, 112, 8, 2399–2404, DOI: https://doi.org/10.1021/jp077583k

44) **Vatamanu J**, Kusalik PG, "Microfaceting and its implication in the nonrandom stacking in fcc crystals", *Phys. Rev. B* **2007**, 76, 035431, DOI: https://doi.org/10.1103/PhysRevB.76.035431

45) **Vatamanu J**, Kusalik PG, "Molecular dynamics methodology to investigate steady-state heterogeneous crystal growth", **2007**, *J. Chem. Phys.* 126, 124703, DOI: https://doi.org/10.1063/1.2710263

46) **Vatamanu J**, Kusalik PG, "Unusual Crystalline and Polycrystalline Structures in Methane Hydrates", *JACS*, **2006**, 128, 49, 15588–15589, DOI: https://doi.org/10.1021/ja066515t

47) **Vatamanu J**, Kusalik PG, "Molecular Insights into the Heterogeneous Crystal Growth of sI Methane Hydrate", *J. Phys. Chem. B.*, **2006**, 110, 32, 15896–15904, DOI: https://doi.org/10.1021/jp061684l

48) **Vatamanu J**, Cann NM, "Evaluation of site-site bridge diagrams for molecular fluids", *J. Chem. Phys.*, **2004**, 110, 32, 15896–15904, DOI: https://doi.org/10.1063/1.1789131

49) **Vatamanu J**, Cressman E, Cann NM, "Discrimination in racemates of small chiral molecules", *Molecular Physics*, **2003**, 101, 3085-3102, DOI: https://doi.org/10.1080/00268970310001614237

50) **Vatamanu J**, Cann NM, " Racemic fluids of hard molecules", *J. Chem. Phys.* **2001**, 114, 7993–8007, DOI: https://doi.org/10.1063/1.1359184

Ph. D. Thesis:

1) **Vatamanu J**, „Atom-Based Integral Equation Theories for Chiral Fluids", Ph.D. Thesis, Queen's University, Kingston, Canada, Ontario. Graduation Year: **2004**,
Link-1: https://library-archives.canada.ca/eng/services/services-libraries/theses/Pages/item.aspx?idNumber=79255277
Link-2: https://bac-lac.on.worldcat.org/oclc/79255277

Book Chapters:

1) Bedrov D, **Vatamanu J**, „ Capacitance with Different Electrode Surface Topology" , In Zhang S., (eds) Enciclopedia of Ionic Liquids, **2022**, pp. 159-167, Springer, Singapore, link: https://link.springer.com/referenceworkentry/10.1007/978-981-33-4221-7_16

2) **Vatamanu J***, Xing L, Bedrov D, „Modeling Methods of Ionic Liquids at Charged Electrode Surfaces", In Zhang S., (eds) Enciclopedia of Ionic Liquids, **2022**, pp. 901-910, Springer, Singapore,
link: https://link.springer.com/referenceworkentry/10.1007/978-981-33-4221-7_114

Conference articles:

1) Borodin O, **Vatamanu J**, Smith G, "Bulk and Interfacial Behavior of Ionic Liquids from Molecular Dynamics Simulations", ECS Trans., **2010**, 33, 583, DOI: 10.1149/1.3484817, link: https://iopscience.iop.org/article/10.1149/1.3484817

2) Gillis K, **Vatamanu J**, Gulam Razul MS, Kusalik PG*, "Averaged configurations from molecular dynamics simulations", CONFERENCE: Applied Parallel Computing. State of the Art in Scientific Computing: 8th International Workshop, PARA 2006, Umeå, Sweden, June 18-21, **2006**, Revised Selected Papers 8, pages: 51-58, Publisher: Springer Berlin Heidelberg,
link: https://link.springer.com/chapter/10.1007/978-3-540-75755-9_6

3) Kusalik PG*, **Vatamanu J**, "A Microscopic View of the Crystal Growth of Gas Hydrates", Open Collections, International Conference on Gas Hydrates (ICGH) (6th : **2008**),
link: https://open.library.ubc.ca/soa/cIRcle/collections/59278/items/1.0041019 ,
DOI: https://dx.doi.org/10.14288/1.0041019

Conferences (more recent, selected):

- Sea-Conf, “On the role of solvent and additive on improving batteries”, Constanta, ANMB, **2024**
- Sea-Conf, “Nanostructure Examinate by Electron Diffraction Using Precession of Electron Beam”, Constanta, ANMB, **2024**
- “Molecular Modeling of Lithium and Zinc Electrolytes”(invited), Electrochemical Society (ECS) **2021**
- “Insight into Aqueous and Non-Aqueous Electrolyte Structure, Transport and Interfacial Properties from Molecular Modeling”(invited), ECS, **2020**
- “Molecular Scale Modeling of Structure, Transport and Electrochemistry of Aqueous and Non-Aqueous Electrolytes” (invited), ECS, **2019**
- "Understanding electrolyte oxidation and reduction at electrode and SEI surfaces", ACS, San Diego, **2019**
- “Recent Progress in Understanding Battery Electrolyte Electrochemical Stability and Its Relationship with Electrolyte Structural Properties”, ECS, **2018**
- “Mesoscale structural and dynamic correlations in ionic liquids sampled by atomistic molecular dynamics simulations”, Chemical Society, **2018**
- “Structure and Transport of ‘Water-in-Salt’ Electrolytes from Molecular Dynamics Simulations”, ECS, National Harbour DC, **2017**

Professional activities and services:

- Part of my recent theoretical research contributed to large collaborative and multidisciplinary projects; an important role of theoretical computations is to provide atomistic insights and mechanisms of the observed experimental phenomena.

- During my participation as a full time Senior Fellow at the Army Research Laboratory Research Associateship Program (ARL-RAP) via ORAU, I was involved in theoretical and computational research on collaborative projects addressing cutting edge solvent-in-salt electrolytes for newer generations of lithium and zinc electrochemical batteries with high energy density and excellent cycle-ability
  Also, I implemented simulation techniques in the legacy MD engine “tinker-hp”, which involved collaboration with Tinker-hp’s software development team.

- I was a research member of the Collaborative Research Alliance (CRA) “Computationally Guided Design of Energy Efficient Electronic Materials” between the University of Utah and the US Army Research Laboratory

- I was involved in a collaborative project with the experimental group of Prof. Yuri Gogotsi from Drexel University about supercapacitors and porous conductive carbon.

- I wrote tens of thousands of lines of code (many in fortran03/08), in-house MD simulation codes, and multiple python scripts.

- I am also did/do (at editor request) peer-review of manuscripts submitted for publication to scientific journals such as *Journal of Physical Chemistry*, *Journal of Chemical Physics*, *Langmuir*, *Journal of Physical Chemistry Letters*, *Electrochimica Acta*, *Fluid Phase Equilibria, Chemical Physics Letters,* and *ACS Nano*

- I wrote manuscript papers for publication in Scientific Journals.

- I wrote parts of research proposals and a research proposal as part of the application for an ORAU fellowship for a Senior Fellow position at ARL-RAP (which I got it).

- I wrote research proposals and parts of research proposal at ANMB.

DATA SEMNATURA

12-IUNIE-2024