

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

LISTA DE LUCRĂRI A Dr. VATAMANU PETRISOR JENEL
 ANUL UNIVERSITAR 2024-2025

1. Lista celor maximum 10 lucrări considerate de candidat a fi cele mai relevante pentru realizările profesionale proprii, care sunt incluse în format electronic în dosar și care se pot regăsi și în celelalte categorii de lucrări prevăzute de prezentul articol:

- Lucrări publicate în reviste Web of Science
- Lucrări în reviste indexate în baze de date
- Lucrări în volume ale manifestărilor științifice internaționale
- Lucrări în volumele manifestărilor științifice naționale

- 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) 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://www.nature.com/articles/s41565-021-00905-4>
- 5) 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>
- 6) 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://pubs.acs.org/doi/full/10.1021/acsenergylett.0c00348>
- 7) 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://www.nature.com/articles/s41467-019-11439-8>

- 8) **Vatamanu J***, Bedrov D “Capacitive Energy Storage: Current and Future Challenges”, (perspective, invited), *Journal of Physical Chemistry Letter*, 2015, 18, 3594-3609 ,
DOI : <https://pubs.acs.org/doi/full/10.1021/acs.jpcllett.5b01199>
- 9) **Vatamanu J**, Kusalik PG* “Observation of two-step nucleation in methane hydrates”, *Phys. Chem. Chem. Phys.*, **2010**, 12, 15065- 15072 ,
DOI : <https://pubs.rsc.org/en/content/articlelanding/2010/cp/c0cp00551g/unauth>
- 10) **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://pubs.acs.org/doi/full/10.1021/ja104273r>

- Lucrări publicate în reviste ISI: Aceste lucrări sunt indexate si apar in SCOPUS.

- 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/acsenerylett.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.jpcclett.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.jpcclett.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.jpcllett.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.jpcllett.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.jnoncrsol.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>

2. Teza sau tezele de doctorat;

- 1) **Vatamanu J**, „Atom-Based Integral Equation Theories for Chiral Fluids”, Ph.D. Thesis, Queen’s University, Kingston, Canada, Ontario. Graduation Year: **2004**, Thesis Advisor: Prof. Dr. Natalie M Cann,
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>

3. Brevete de invenție și alte titluri de proprietate industrială;

4. Cărți și capitole în cărți;

- 1) Bedrov D, **Vatamanu J**, „Capacitance with Different Electrode Surface Topology” , In Zhang S., (eds) Encyclopedia 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) Encyclopedia of Ionic Liquids, **2022**, pp. 901-910, Springer, Singapore,
link: https://link.springer.com/referenceworkentry/10.1007/978-981-33-4221-7_114

5. Articole/studii in extenso, publicate în reviste din fluxul științific internațional principal

(vezi lista de 50 de articole ISI de mai sus)

6. Publicații in extenso, apărute în lucrări ale principalelor conferințe internaționale de specialitate

- 1) Borodin O, **Vatamanu J**, Smith G, "Bulk and Interfacial Behavior of Ionic Liquids from Molecular Dynamics Simulations", ECS Trans., 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>

7. Contracte/proiecte de cercetare-dezvoltare-inovare pe bază de contract/grant (incluzând numele proiectului, codul, competiția, directorul de proiect, valoarea totală, valoarea alocată instituției membre la care candidatul era afiliat în timpul derulării proiectului, alte informații)

7.A. Proiecte la care eu sunt P.I. (sunt proiecte de acces la resurse la supercomputerele Europei via EuroHPC):

- 1) "Implementation of polarizable force fields via inducible dipoles in LAMMPS general purpose parallel molecular dynamics code", PI, Euro-HPC, <https://pracecalls.eu/applications/EHPC-DEV-2023D12-075> (project to be granted access to computing resources via the calls at: https://eurohpc-ju.europa.eu/access-our-supercomputers/eurohpc-access-calls_en)
- 2) "Implementation of atomic-level anisotropy polarizable force-fields into TINKER-HP and LAMMPS general purpose parallel molecular dynamics codes", PI, Euro-HPC, <https://pracecalls.eu/applications/EHPC-DEV-2023D12-009> (project to be granted access to computing resources)
- 3) "Benchmarking molecular dynamics simulation community codes LAMMPS, GROMACS, OpenMM, CP2K, on EuroHPC super-computer.", PI, Euro-HPC, <https://pracecalls.eu/applications/EHPC-BEN-2023B12-006> (project to be granted access to computing resources)

7.B. Contracte la care eu nu am fost nici P.I. si nici co-P.I. dar care au suportat cercetarea făcută de mine:

- 1) Pe durata postdocului in Canada la Dalhousie Univ. si University of Calgary, Advisor & PI: Prof. Peter G Kusalik (copy/paste din scrisoarea de verificare) :

His work with my research group was support by the following funding:

| Name(s) | Funding agency, type of support, title, ... | Amount (/yr) | Tenure |
|---------------------------|---|--|--------------------------------------|
| P.G. Kusalik | University of Calgary, Startup Funding | \$150,000 | 2005/06 |
| P.G. Kusalik | Natural Sciences and Engineering Research Council (NSERC). Research Grant. "Computer Simulation Studies of Molecular Liquids, Solutions and Crystallization." | \$50,000 | 2001/02 to 2005/06 |
| P.G. Kusalik and others | C3.ca Technical Analyst Support Program (TASP) for Dalhousie University (ACENET) | \$22,000 | 2004/05 |
| P.G. Kusalik | Research grant (Faculty of Science) negotiated as part of arrangement in being Acting Associate Dean | \$10,000 | 2004/05 |
| As co-investigator | | | |
| M.A. White with 12 others | Atlantic Innovations Fund. "Materials Technology Network for Atlantic Canada" | \$5,000,000 (3%) \$350,000 (15%) \$350,000 (15%) \$350,000 (15%) \$350,000 (15%) | 2003 2004 2005 2006 2007 |
| M.A. White with 23 others | NSERC. Major Facilities Access. "Materials Characterization Facilities" | \$133,000 (8%) \$160,000 (6%) \$160,000 (6%) | 2003 2004 2005 |
| M.A. White with 8 others | Canada Foundation for Innovation (CFI) plus industrial partners. "Facilities for Materials Characterization" | \$4,800,000 (3%) \$400,000 (0%) | 2003 2004 |

- 2) Pe durata Jobului de Cercetator Asociat din University of Utah (Advisors Dr. Grant D Smith (initial) si Dr. D. Bedrov): (copy/paste din emailul de confirmare)

- 1) DOE-SISGR "Influence of electrolyte structure and electrode morphology on the performance of ionic liquid based supercapacitors" (DECS00001912), 2009-2013, project budget \$1,500,000, PIs: Grant D. Smith and Dmitry Bedrov.
- 2) DOD "Collaborative Research Alliance for Multiscale Modeling of Electronic Materials" (W911NF-12-2-0023), 2012-2021, budget \$1,900,000, PI: Dmitry Bedrov.

- 3) Pe durata participării ca full-time senior fellow la programul ARL-RAP via ORAU: (copy/paste din scrisoarea de verificare):

Dr. Vatamanu's participation was full time during which time he worked on several projects supported by:

- Department of Energy through Joint Center for Energy Storage Research from 06/2017 - 2022, PI for ARL part, Kang Xu, \$500K/year
- ARL Directors Research Initiative on Modeling Electrodeposition, 2016 – 2019, PI Oleg Borodin, \$200K/year
- Department of Energy, Understanding Cathode – Electrolyte Interfaces, 2019-2020, co-PI Oleg Borodin, 125K/year

8. Alte lucrări și contribuții științifice sau, după caz, din domeniul creației artistice.

- 1) Am creat cover-ul, adica imaginea de pe coperta, la jurnalul „Journal of Physical Chemistry Letters”, **2015**, September 17, Volume 6, Issue 18. In procesul creării acelu cover am avut feed-back de la Dr. Dmitry Bedrov si de la Dr. Mihaela Vatamanu.
Link catre volumul in cauza (cu cover-ul respectiv): <https://pubs.acs.org/toc/jpclcd/6/18>

Data

Semnătura

11-JUNE-2024



