

# Vladislav B IvaniĀ;tĀ;ev

## List of Publications by Year in descending order

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42  
papers

1,004  
citations

394421

19  
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454955

30  
g-index

44  
all docs

44  
docs citations

44  
times ranked

1061  
citing authors

#	ARTICLE	IF	CITATIONS
1	Catalytic CO <sub>2</sub> /CO Reduction: Gas, Aqueous, and Aprotic Phases. ACS Catalysis, 2022, 12, 2561-2568.	11.2	22
2	Double layer in ionic liquids: Temperature effect and bilayer model. Journal of Molecular Liquids, 2022, 363, 119747.	4.9	10
3	Ionic liquid-metal interface: The origins of capacitance peaks. Electrochimica Acta, 2021, 379, 138148.	5.2	28
4	Multifunctional Electrocatalysis on Single-Site Metal Catalysts: A Computational Perspective. Catalysts, 2021, 11, 1165.	3.5	11
5	Graphene-Ionic Liquid Interfacial Potential Drop from Density Functional Theory-Based Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2020, 124, 19548-19555.	3.1	24
6	Calculation of core-level electron spectra of ionic liquids. International Journal of Quantum Chemistry, 2020, 120, e26247.	2.0	3
7	Understanding the Behavior of Fully Non-Toxic Polypyrrole-Gelatin and Polypyrrole-PVdF Soft Actuators with Choline Ionic Liquids. Actuators, 2020, 9, 40.	2.3	10
8	Hysteresis in the MD Simulations of Differential Capacitance at the Ionic Liquid-Au Interface. Journal of Physical Chemistry Letters, 2020, 11, 10408-10413.	4.6	14
9	Simulation of a Solvate Ionic Liquid at a Polarizable Electrode with a Constant Potential. Journal of Physical Chemistry C, 2019, 123, 3935-3943.	3.1	16
10	On the role of the surface charge plane position at Au(hkl)-BMIImPF6 interfaces. Electrochimica Acta, 2019, 318, 76-82.	5.2	15
11	Molecular dynamics simulations of novel electrolytes based on mixtures of protic and aprotic ionic liquids at the electrochemical interface: Structure and capacitance of the electric double layer. Electrochimica Acta, 2019, 305, 223-231.	5.2	16
12	Predicting Melting Points of Biofriendly Choline-Based Ionic Liquids with Molecular Dynamics. Applied Sciences (Switzerland), 2019, 9, 5367.	2.5	7
13	Density Functional Theory Study of Ionic Liquid Adsorption on Circumcoronene Shaped Graphene. Journal of Physical Chemistry C, 2018, 122, 2624-2631.	3.1	26
14	Performance of SCAN density functional for a set of ionic liquid ion pairs. International Journal of Quantum Chemistry, 2018, 118, e25582.	2.0	10
15	On the thickness of the double layer in ionic liquids. Physical Chemistry Chemical Physics, 2018, 20, 10275-10285.	2.8	40
16	Structure and dynamics of ionic liquids: general discussion. Faraday Discussions, 2018, 206, 291-337.	3.2	8
17	Ionic liquids at interfaces: general discussion. Faraday Discussions, 2018, 206, 549-586.	3.2	0
18	NaRiBa-A Scripting Framework for Computational Modeling of Nanomaterials and Room Temperature Ionic Liquids in Bulk and Slab. Computation, 2018, 6, 57.	2.0	7

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19	The nanostructure of a lithium glyme solvate ionic liquid at electrified interfaces. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 11004-11010.	2.8	27
20	Molecular dynamics simulation of the structure and interfacial free energy barriers of mixtures of ionic liquids and divalent salts near a graphene wall. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 846-853.	2.8	33
21	Predictions of Physicochemical Properties of Ionic Liquids with DFT. <i>Computation</i> , 2016, 4, 25.	2.0	35
22	Electrochemical Investigation of 1-Ethyl-3-methylimidazolium Bromide and Tetrafluoroborate Mixture at Bi(111) Electrode Interface. <i>Journal of the Electrochemical Society</i> , 2016, 163, H723-H730.	2.9	26
23	Interplay between the hydrophilicity of metal electrodes and their interfacial capacitance. <i>Electrochimica Acta</i> , 2016, 210, 615-621.	5.2	8
24	Molecular dynamics simulation of the behaviour of water in nano-confined ionic liquid-water mixtures. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 464001.	1.8	44
25	Characteristics of Capacitors Based on Ionic Liquids: From Dielectric Polymers to Redox-Active Adsorbed Species. <i>ECS Transactions</i> , 2016, 75, 161-170.	0.5	6
26	Self-interaction error in DFT-based modelling of ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 2175-2182.	2.8	20
27	Molecular origin of high free energy barriers for alkali metal ion transfer through ionic liquid-graphene electrode interfaces. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1302-1310.	2.8	39
28	Restructuring of the electrical double layer in ionic liquids upon charging. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 102101.	1.8	37
29	Adsorption of 4,4'-bipyridine on the Cd(0001) single crystal electrode surface. <i>Electrochimica Acta</i> , 2015, 180, 965-976.	5.2	10
30	Molecular Response of 1-Butyl-3-Methylimidazolium Dicyanamide Ionic Liquid at the Graphene Electrode Interface Investigated by Sum Frequency Generation Spectroscopy and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2015, 119, 26009-26019.	3.1	44
31	Balance of the interfacial interactions of 4,4'-bipyridine at Bi(111) surface. <i>Electrochimica Acta</i> , 2014, 120, 86-95.	5.2	15
32	Poly(amorphous) portrait of the electrical double layer in ionic liquids. <i>Electrochemistry Communications</i> , 2014, 48, 61-64.	4.7	64
33	Screening of Ion-Graphene Electrode Interactions by Ionic Liquids: The Effects of Liquid Structure. <i>Journal of Physical Chemistry C</i> , 2014, 118, 5841-5847.	3.1	54
34	Interfaces between Charged Surfaces and Ionic Liquids: Insights from Molecular Simulations. <i>Electrochemical Society Interface</i> , 2014, 23, 65-69.	0.4	45
35	Comparative Impedance Study of Cd(0001) Electrode in EMImBF <sub>4</sub> and KI Aqueous Solution at Different Temperatures. <i>Journal of the Electrochemical Society</i> , 2013, 160, H368-H375.	2.9	18
36	Direct migration of scientific computing experiments to the cloud. , 2013, , .		3

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37	A comparative DFT study of the adsorption of H <sub>2</sub> O molecules at Bi, Hg, and Ga surfaces. <i>Surface Science</i> , 2013, 609, 91-99.	1.9	14
38	Electrical double layer in ionic liquids: Structural transitions from multilayer to monolayer structure at the interface. <i>Electrochimica Acta</i> , 2013, 110, 762-771.	5.2	110
39	Influence of the electrode potential and in situ STM scanning conditions on the phase boundary structure of the single crystal Bi(1 1 1)   1-butyl-4-methylpyridinium tetrafluoroborate interface. <i>Journal of Electroanalytical Chemistry</i> , 2013, 709, 46-56.	3.8	22
40	Influence of cation chemical composition and structure on the double layer capacitance for Bi(111)   room temperature ionic liquid interface. <i>Journal of Electroanalytical Chemistry</i> , 2012, 668, 30-36.	3.8	43
41	Impedance study of adsorption of iodide ions at Cd(0001) and Bi(111) electrode from various solutions with constant ionic strength. <i>Journal of Solid State Electrochemistry</i> , 2010, 14, 555-563.	2.5	4
42	Density functional theory study of the water adsorption at Bi(111) electrode surface. <i>Surface Science</i> , 2010, 604, 1919-1927.	1.9	16