

# Maxim V Ivanov

## List of Publications by Year in descending order

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48  
papers

1,220  
citations

566801

15  
h-index

395343

33  
g-index

52  
all docs

52  
docs citations

52  
times ranked

1232  
citing authors

#	ARTICLE	IF	CITATIONS
1	Mechanism-Based Inactivation of Cytochrome P450 Enzymes: Computational Insights. <i>Chemical Research in Toxicology</i> , 2021, 34, 959-987.	1.7	11
2	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
3	Toward Ultracold Organic Chemistry: Prospects of Laser Cooling Large Organic Molecules. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 6670-6676.	2.1	26
4	In search of molecular ions for optical cycling: a difficult road. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 17075-17090.	1.3	20
5	Long-Range Nâ€“N Bonding by Rydberg Electrons. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 2284-2290.	2.1	8
6	Two Cycling Centers in One Molecule: Communication by Through-Bond Interactions and Entanglement of the Unpaired Electrons. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 1297-1304.	2.1	25
7	Improving Performance of the SMD Solvation Model: Bondi Radii Improve Predicted Aqueous Solvation Free Energies of Ions and $pK_a$ Values of Thiols. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9498-9504.	1.1	37
8	Towards a rational design of laser-coolable molecules: insights from equation-of-motion coupled-cluster calculations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 19447-19457.	1.3	36
9	Charge-transfer or excimeric state? Exploring the nature of the excited state in cofacially arrayed polyfluorene derivatives. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 374, 125-130.	2.0	2
10	From Intramolecular (Circular) in an Isolated Molecule to Intermolecular Hole Delocalization in a Twoâ€“Dimensional Solidâ€“State Assembly: The Case of Pillarene. <i>Angewandte Chemie</i> , 2018, 130, 2166-2171.	1.6	1
11	Strength of $\pi$ -Stacking, from Neutral to Cation: Precision Measurement of Binding Energies in an Isolated $\pi$ -Stacked Dimer. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 2058-2061.	2.1	15
12	Probing Charge Delocalization in Solid State Polychromophoric Cation Radicals Using X-ray Crystallography and DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2018, 122, 9339-9345.	1.5	6
13	Ask Not How Many, But Where They Are: Substituents Control Energetic Ordering of Frontier Orbitals/Electronic Structures in Isomeric Methoxy-Substituted Dibenzochrysenes. <i>Journal of Physical Chemistry C</i> , 2018, 122, 2539-2545.	1.5	19
14	FHBC, a Hexaâ€“periâ€“hexabenzocoroneneâ€“Fluorene Hybrid: A Platform for Highly Soluble, Easily Functionalizable HBCs with an Expanded Graphitic Core. <i>Angewandte Chemie</i> , 2018, 130, 798-802.	1.6	5
15	From Intramolecular (Circular) in an Isolated Molecule to Intermolecular Hole Delocalization in a Twoâ€“Dimensional Solidâ€“State Assembly: The Case of Pillarene. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 2144-2149.	7.2	8
16	From Static to Dynamic: Electron Density of HOMO at Biaryl Linkage Controls the Mechanism of Hole Delocalization. <i>Journal of the American Chemical Society</i> , 2018, 140, 4765-4769.	6.6	11
17	FHBC, a Hexaâ€“periâ€“hexabenzocoroneneâ€“Fluorene Hybrid: A Platform for Highly Soluble, Easily Functionalizable HBCs with an Expanded Graphitic Core. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 790-794.	7.2	12
18	Reactive pathways in the bromobenzene-ammonia dimer cation radical: Evidence for a roaming halogen radical. <i>Journal of Molecular Structure</i> , 2018, 1172, 113-118.	1.8	2

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19	Vertical vs. adiabatic ionization energies in solution and gas-phase: probing ionization-induced reorganization in conformationally-mobile bichromophoric actuators using photoelectron spectroscopy, electrochemistry and theory. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 25615-25622.	1.3	9
20	Dynamic Phosphorylation of the C Terminus of Hsp70 Regulates the Mitochondrial Import of SOD2 and Redox Balance. <i>Cell Reports</i> , 2018, 25, 2605-2616.e7.	2.9	40
21	π-π stacking vs. C-H...H interaction: Excimer formation and charge resonance stabilization in van der Waals clusters of 9,9-dimethylfluorene. <i>Journal of Chemical Physics</i> , 2018, 149, 134314.	1.2	10
22	An Electron-Rich Calix[4]arene-Based Receptor with Unprecedented Binding Affinity for Nitric Oxide. <i>Chemistry - A European Journal</i> , 2018, 24, 17439-17443.	1.7	6
23	Pyrene-Like HOMO Governs Polaron Delocalization in Model Graphitic Strips: A Combined Experimental and Computational Analysis. <i>Journal of Physical Chemistry C</i> , 2018, 122, 24527-24534.	1.5	1
24	Game of Frontier Orbitals: A View on the Rational Design of Novel Charge-Transfer Materials. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3978-3986.	2.1	25
25	An electron-transfer induced conformational transformation: from non-cofacial π-π to cofacial π-π in cyclotetraarylene (CTTV) and formation of charge transfer complexes. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 5712-5717.	1.5	9
26	Molecular Actuators in Action: Electron-Transfer-Induced Conformation Transformation in Cofacially Arrayed Polyfluorenes. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4233-4238.	2.1	7
27	Spreading Electron Density Thin: Increasing the Chromophore Size in Polyaromatic Wires Decreases Interchromophoric Electronic Coupling. <i>Journal of Physical Chemistry C</i> , 2018, 122, 17668-17675.	1.5	7
28	The Role of Torsional Dynamics on Hole and Exciton Stabilization in π-π Stacked Assemblies: Design of Rigid Torsionomers of a Cofacial Bifluorene. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 8189-8193.	7.2	16
29	The Role of Torsional Dynamics on Hole and Exciton Stabilization in π-π Stacked Assemblies: Design of Rigid Torsionomers of a Cofacial Bifluorene. <i>Angewandte Chemie</i> , 2018, 130, 8321-8325.	1.6	4
30	Towards the rational design of novel charge-transfer materials: biaryls with a dihedral angle-independent hole delocalization mechanism. <i>Chemical Communications</i> , 2018, 54, 5851-5854.	2.2	5
31	Hückel Theory + Reorganization Energy = Marcus-Hush Theory: Breakdown of the 1/n Trend in π-Conjugated Poly(p-phenylene) Cation Radicals Is Explained. <i>Journal of Physical Chemistry C</i> , 2017, 121, 1552-1561.	1.5	27
32	Poly(p-hydroquinone) Ethers: Isoenergetic Molecular Wires with Length-Invariant Oxidation Potentials and Cation Radical Excitation Energies. <i>Journal of the American Chemical Society</i> , 2017, 139, 4334-4337.	6.6	16
33	Isolation of a chiral anthracene cation radical: X-ray crystallography and computational interrogation of its racemization. <i>Chemical Communications</i> , 2017, 53, 2748-2751.	2.2	7
34	Nodal Arrangement of HOMO Controls the Turning On/Off the Electronic Coupling in Isomeric Polypyrene Wires. <i>Journal of Physical Chemistry C</i> , 2017, 121, 9202-9208.	1.5	14
35	Dihedral-Angle-Controlled Crossover from Static Hole Delocalization to Dynamic Hopping in Biaryl Cation Radicals. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 266-269.	7.2	12
36	Dihedral-Angle-Controlled Crossover from Static Hole Delocalization to Dynamic Hopping in Biaryl Cation Radicals. <i>Angewandte Chemie</i> , 2017, 129, 272-275.	1.6	7

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37	Unraveling the Coulombic Forces in Electronically Decoupled Bichromophoric Systems during Two Successive Electron Transfers. <i>Chemistry - A European Journal</i> , 2017, 23, 8834-8838.	1.7	8
38	Cofacially Arrayed Polyfluorenes: Spontaneous Formation of $\pi$ -Stacked Assemblies in the Gas Phase. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5272-5276.	2.1	9
39	When Substituents Do Not Matter: Frontier Orbitals Explain the Unusually High and Invariant Oxidation Potential in Alkoxy-, Alkyl-, and H-Substituted Iptycenes. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4226-4230.	2.1	7
40	Through-Space or Through-Bond? The Important Role of Cofaciality in Orbital Reordering and Its Implications for Hole (De)stabilization in Polychromophoric Assemblies. <i>Journal of Physical Chemistry C</i> , 2017, 121, 15639-15643.	1.5	6
41	Effect of Facial Encumbrance on Excimer Formation and Charge Resonance Stabilization in Model Bichromophoric Assemblies. <i>Journal of Physical Chemistry C</i> , 2017, 121, 15580-15588.	1.5	10
42	First Experimental Evidence for the Diverse Requirements of Excimer vs Hole Stabilization in $\pi$ -Stacked Assemblies. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3042-3045.	2.1	14
43	Two's Company, Three's a Crowd: Exciton Localization in Cofacially Arrayed Polyfluorenes. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2915-2920.	2.1	12
44	Energy Gap between the Poly-p-phenylene Bridge and Donor Groups Controls the Hole Delocalization in Donor-Bridge-Donor Wires. <i>Journal of the American Chemical Society</i> , 2016, 138, 16337-16344.	6.6	29
45	Inclusion of Asymptotic Dependence of Reorganization Energy in the Modified Marcus-Based Multistate Model Accurately Predicts Hole Distribution in Poly-p-phenylene Wires. <i>Journal of Physical Chemistry C</i> , 2016, 120, 6402-6408.	1.5	18
46	Electrostatic point charge fitting as an inverse problem: Revealing the underlying ill-conditioning. <i>Journal of Chemical Physics</i> , 2015, 143, 134102.	1.2	5
47	Genetic Algorithm Optimization of Point Charges in Force Field Development: Challenges and Insights. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1422-1434.	1.1	24
48	Electronic structure of $\hat{\Gamma}$ -Ta <sub>2</sub> O <sub>5</sub> with oxygen vacancy: <i>ab initio</i> calculations and comparison with experiment. <i>Journal of Applied Physics</i> , 2011, 110, .	1.1	94