Maxim V Ivanov

List of Publications by Year
in descending order

48	1,220	566801 15	395343 33
papers	citations	h-index	g-index

52	52	52	1232
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
2	Electronic structure of Î´-Ta2O5 with oxygen vacancy: ab initio calculations and comparison with experiment. Journal of Applied Physics, 2011, 110, .	1.1	94
3	Dynamic Phosphorylation of the C Terminus of Hsp70 Regulates the Mitochondrial Import of SOD2 and Redox Balance. Cell Reports, 2018, 25, 2605-2616.e7.	2.9	40
4	Improving Performance of the SMD Solvation Model: Bondi Radii Improve Predicted Aqueous Solvation Free Energies of Ions and pK_a Values of Thiols. Journal of Physical Chemistry A, 2019, 123, 9498-9504.	1.1	37
5	Towards a rational design of laser-coolable molecules: insights from equation-of-motion coupled-cluster calculations. Physical Chemistry Chemical Physics, 2019, 21, 19447-19457.	1.3	36
6	Energy Gap between the Poly-p-phenylene Bridge and Donor Groups Controls the Hole Delocalization in Donorâ€“Bridgeâ€“Donor Wires. Journal of the American Chemical Society, 2016, 138, 16337-16344.	6.6	29
7	HÃ¼ckel Theory + Reorganization Energy = Marcusâ€“Hush Theory: Breakdown of the 1/n Trend in Ï€-Conjugated Poly-p-phenylene Cation Radicals Is Explained. Journal of Physical Chemistry C, 2017, 121, 1552-1561.	1.5	27
8	Toward Ultracold Organic Chemistry: Prospects of Laser Cooling Large Organic Molecules. Journal of Physical Chemistry Letters, 2020, 11, 6670-6676.	2.1	26
9	Game of Frontier Orbitals: A View on the Rational Design of Novel Charge-Transfer Materials. Journal of Physical Chemistry Letters, 2018, 9, 3978-3986.	2.1	25
10	Two Cycling Centers in One Molecule: Communication by Through-Bond Interactions and Entanglement of the Unpaired Electrons. Journal of Physical Chemistry Letters, 2020, 11, 1297-1304.	2.1	25
11	Genetic Algorithm Optimization of Point Charges in Force Field Development: Challenges and Insights. Journal of Physical Chemistry A, 2015, 119, 1422-1434.	1.1	24
12	In search of molecular ions for optical cycling: a difficult road. Physical Chemistry Chemical Physics, 2020, 22, 17075-17090.	1.3	20
13	Ask Not How Many, But Where They Are: Substituents Control Energetic Ordering of Frontier Orbitals/Electronic Structures in Isomeric Methoxy-Substituted Dibenzochrysenes. Journal of Physical Chemistry C, 2018, 122, 2539-2545.	1.5	19
14	Inclusion of Asymptotic Dependence of Reorganization Energy in the Modified Marcus-Based Multistate Model Accurately Predicts Hole Distribution in Poly-p-phenylene Wires. Journal of Physical Chemistry C, 2016, 120, 6402-6408.	1.5	18
15	Poly-p-hydroquinone Ethers: Isoenergetic Molecular Wires with Length-Invariant Oxidation Potentials and Cation Radical Excitation Energies. Journal of the American Chemical Society, 2017, 139, 4334-4337.	6.6	16
16	The Role of Torsional Dynamics on Hole and Exciton Stabilization in Ï€â€Stacked Assemblies: Design of Rigid Torsionomers of a Cofacial Bifluorene. Angewandte Chemie - International Edition, 2018, 57, 8189-8193.	7.2	16
17	Strength of Ï€-Stacking, from Neutral to Cation: Precision Measurement of Binding Energies in an Isolated Ï€-Stacked Dimer. Journal of Physical Chemistry Letters, 2018, 9, 2058-2061.	2.1	15
18	First Experimental Evidence for the Diverse Requirements of Excimer vs Hole Stabilization in Ï€-Stacked Assemblies. Journal of Physical Chemistry Letters, 2016, 7, 3042-3045.	2.1	14

#	Article	IF	Citations
19	Nodal Arrangement of HOMO Controls the Turning On/Off the Electronic Coupling in Isomeric Polypyrene Wires. Journal of Physical Chemistry C, 2017, 121, 9202-9208.	1.5	14
20	Twoâ€™s Company, Threeâ€™s a Crowd: Exciton Localization in Cofacially Arrayed Polyfluorenes. Journal of Physical Chemistry Letters, 2016, 7, 2915-2920.	2.1	12
21	Dihedralâ€Angleâ€Controlled Crossover from Static Hole Delocalization to Dynamic Hopping in Biaryl Cation Radicals. Angewandte Chemie - International Edition, 2017, 56, 266-269.	7.2	12
22	FHBC, a Hexaâ€periâ€hexabenzocoroneneâ€“Fluorene Hybrid: A Platform for Highly Soluble, Easily Functionalizable HBCs with an Expanded Graphitic Core. Angewandte Chemie - International Edition, 2018, 57, 790-794.	7.2	12
23	From Static to Dynamic: Electron Density of HOMO at Biaryl Linkage Controls the Mechanism of Hole Delocalization. Journal of the American Chemical Society, 2018, 140, 4765-4769.	6.6	11
24	Mechanism-Based Inactivation of Cytochrome P450 Enzymes: Computational Insights. Chemical Research in Toxicology, 2021, 34, 959-987.	1.7	11
25	Effect of Facial Encumbrance on Excimer Formation and Charge Resonance Stabilization in Model Bichromophoric Assemblies. Journal of Physical Chemistry C, 2017, 121, 15580-15588.	1.5	10
26	Ï€-Ï€ stacking vs. Câ€“H/Ï€ interaction: Excimer formation and charge resonance stabilization in van der Waals clusters of 9,9â€²-dimethylfluorene. Journal of Chemical Physics, 2018, 149, 134314.	1.2	10
27	Cofacially Arrayed Polyfluorenes: Spontaneous Formation of Ï€-Stacked Assemblies in the Gas Phase. Journal of Physical Chemistry Letters, 2017, 8, 5272-5276.	2.1	9
28	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. Physical Chemistry Chemical Physics, 2018, 20, 25615-25622.	1.3	9
29	An electron-transfer induced conformational transformation: from non-cofacial â€œsofaâ€• to cofacial â€œboatâ€• in cyclotetraveratrylene (CTTV) and formation of charge transfer complexes. Organic and Biomolecular Chemistry, 2018, 16, 5712-5717.	1.5	9
30	Unraveling the Coulombic Forces in Electronically Decoupled Bichromophoric Systems during Two Successive Electron Transfers. Chemistry - A European Journal, 2017, 23, 8834-8838.	1.7	8
31	From Intramolecular (Circular) in an Isolated Molecule to Intermolecular Hole Delocalization in a Twoâ€Dimensional Solidâ€State Assembly: The Case of Pillarene. Angewandte Chemie - International Edition, 2018, 57, 2144-2149.	7.2	8
32	Long-Range Nâ€“N Bonding by Rydberg Electrons. Journal of Physical Chemistry Letters, 2020, 11, 2284-2290.	2.1	8
33	Isolation of a chiral anthracene cation radical: X-ray crystallography and computational interrogation of its racemization. Chemical Communications, 2017, 53, 2748-2751.	2.2	7
34	Dihedralâ€Angleâ€Controlled Crossover from Static Hole Delocalization to Dynamic Hopping in Biaryl Cation Radicals. Angewandte Chemie, 2017, 129, 272-275.	1.6	7
35	When Substituents Do Not Matter: Frontier Orbitals Explain the Unusually High and Invariant Oxidation Potential in Alkoxy-, Alkyl-, and H-Substituted Iptycenes. Journal of Physical Chemistry Letters, 2017, 8, 4226-4230.	2.1	7
36	Molecular Actuators in Action: Electron-Transfer-Induced Conformation Transformation in Cofacially Arrayed Polyfluorenes. Journal of Physical Chemistry Letters, 2018, 9, 4233-4238.	2.1	7

#	Article	IF	Citations
37	Spreading Electron Density Thin: Increasing the Chromophore Size in Polyaromatic Wires Decreases Interchromophoric Electronic Coupling. Journal of Physical Chemistry C, 2018, 122, 17668-17675.	1.5	7
38	Through-Space or Through-Bond? The Important Role of Cofaciality in Orbital Reordering and Its Implications for Hole (De)stabilization in Polychromophoric Assemblies. Journal of Physical Chemistry C, 2017, 121, 15639-15643.	1.5	6
39	Probing Charge Delocalization in Solid State Polychromophoric Cation Radicals Using X-ray Crystallography and DFT Calculations. Journal of Physical Chemistry C, 2018, 122, 9339-9345.	1.5	6
40	An Electronâ€Rich Calix[4]areneâ€Based Receptor with Unprecedented Binding Affinity for Nitric Oxide. Chemistry - A European Journal, 2018, 24, 17439-17443.	1.7	6
41	Electrostatic point charge fitting as an inverse problem: Revealing the underlying ill-conditioning. Journal of Chemical Physics, 2015, 143, 134102.	1.2	5
42	FHBC, a Hexaâ€•peri â€hexabenzocoroneneâ€“Fluorene Hybrid: A Platform for Highly Soluble, Easily Functionalizable HBCs with an Expanded Graphitic Core. Angewandte Chemie, 2018, 130, 798-802.	1.6	5
43	Towards the rational design of novel charge-transfer materials: biaryls with a dihedral angle-independent hole delocalization mechanism. Chemical Communications, 2018, 54, 5851-5854.	2.2	5
44	The Role of Torsional Dynamics on Hole and Exciton Stabilization in Ï€â€Stacked Assemblies: Design of Rigid Torsionomers of a Cofacial Bifluorene. Angewandte Chemie, 2018, 130, 8321-8325.	1.6	4
45	Reactive pathways in the bromobenzene-ammonia dimer cation radical: Evidence for a roaming halogen radical. Journal of Molecular Structure, 2018, 1172, 113-118.	1.8	2
46	Charge-transfer or excimeric state? Exploring the nature of the excited state in cofacially arrayed polyfluorene derivatives. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 374, 125-130.	2.0	2
47	From Intramolecular (Circular) in an Isolated Molecule to Intermolecular Hole Delocalization in a Twoâ€Dimensional Solidâ€State Assembly: The Case of Pillarene. Angewandte Chemie, 2018, 130, 2166-2171.	1.6	1
48	Pyrene-Like HOMO Governs Polaron Delocalization in Model Graphitic Strips: A Combined Experimental and Computational Analysis. Journal of Physical Chemistry C, 2018, 122, 24527-24534.	1.5	1