Sergei Manzhos

List of Publications by Year
in descending order

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Version: 2024-02-01

216 papers	6,173 citations	61945 43 h-index	98753 67 g-index
224 all docs	224 docs citations	224 times ranked	5814 citing authors

#	Article	IF	Citations
1	A random-sampling high dimensional model representation neural network for building potential energy surfaces. Journal of Chemical Physics, 2006, 125, 084109.	1.2	211
2	Organic interfacial materials for perovskite-based optoelectronic devices. Energy and Environmental Science, 2019, 12, 1177-1209.	15.6	185
3	Neural networkâ€based approaches for building high dimensional and quantum dynamicsâ€friendly potential energy surfaces. International Journal of Quantum Chemistry, 2015, 115, 1012-1020.	1.0	170
4	A Nested Molecule-Independent Neural Network Approach for High-Quality Potential Fitsâ€. Journal of Physical Chemistry A, 2006, 110, 5295-5304.	1.1	166
5	Neural Network Potential Energy Surfaces for Small Molecules and Reactions. Chemical Reviews, 2021, 121, 10187-10217.	23.0	163
6	Neural networks vs Gaussian process regression for representing potential energy surfaces: A comparative study of fit quality and vibrational spectrum accuracy. Journal of Chemical Physics, 2018, 148, 241702.	1.2	157
7	Using neural networks to represent potential surfaces as sums of products. Journal of Chemical Physics, 2006, 125, 194105.	1.2	156
8	Molecular Engineering Using an Anthanthrone Dye for Lowâ€Cost Hole Transport Materials: A Strategy for Dopantâ€Free, Highâ€Efficiency, and Stable Perovskite Solar Cells. Advanced Energy Materials, 2018, 8, 1703007.	10.2	154
9	In search of high performance anode materials for Mg batteries: Computational studies of Mg in Ge, Si, and Sn. Journal of Power Sources, 2013, 233, 341-345.	4.0	103
10	Using neural networks, optimized coordinates, and high-dimensional model representations to obtain a vinyl bromide potential surface. Journal of Chemical Physics, 2008, 129, 224104.	1.2	100
11	Phenothiazine and carbazole substituted pyrene based electroluminescent organic semiconductors for OLED devices. Journal of Materials Chemistry C, 2016, 4, 1009-1018.	2.7	99
12	Using redundant coordinates to represent potential energy surfaces with lower-dimensional functions. Journal of Chemical Physics, 2007, 127, 014103.	1.2	93
13	A computational study of Na behavior on graphene. Applied Surface Science, 2015, 333, 235-243.	3.1	90
14	A Comparative Computational Study of Structures, Diffusion, and Dopant Interactions between Li and Na Insertion into Si. Applied Physics Express, 2013, 6, 027301.	1.1	87
15	Insertion energetics of lithium, sodium, and magnesium in crystalline and amorphous titanium dioxide: A comparative first-principles study. Journal of Power Sources, 2015, 278, 197-202.	4.0	83
16	On the Charge State of Titanium in Titanium Dioxide. Journal of Physical Chemistry Letters, 2017, 8, 1593-1598.	2.1	77
17	Study of Interfacial Charge Transfer Bands and Electron Recombination in the Surface Complexes of TCNE, TCNQ, and TCNAQ with TiO₂. Journal of Physical Chemistry C, 2011, 115, 21487-21493.	1.5	76
18	A computational study of the insertion of Li, Na, and Mg atoms into Si(111) nanosheets. Nano Energy, 2013, 2, 1149-1157.	8.2	76

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19	Controlling Na diffusion by rational design of Si-based layered architectures. Physical Chemistry Chemical Physics, 2014, 16, 4260.	1.3	75
20	Allâ€Rounder Lowâ€Cost Dopantâ€Free Dâ€Aâ€D Holeâ€Transporting Materials for Efficient Indoor and Outdoor Performance of Perovskite Solar Cells. Advanced Electronic Materials, 2020, 6, 1900884.	2.6	72
21	Comparative computational study of the energetics of Li, Na, and Mg storage in amorphous and crystalline silicon. Computational Materials Science, 2014, 94, 214-217.	1.4	70
22	Dopant-free novel hole-transporting materials based on quinacridone dye for high-performance and humidity-stable mesoporous perovskite solar cells. Journal of Materials Chemistry A, 2019, 7, 5315-5323.	5.2	70
23	Roadmap on Machine learning in electronic structure. Electronic Structure, 2022, 4, 023004.	1.0	69
24	Achieving High Efficiency in Solution-Processed Perovskite Solar Cells Using C₆₀/C₇₀ Mixed Fullerenes. ACS Applied Materials & Interfaces, 2018, 10, 39590-39598.	4.0	67
25	Comparison of Li, Na, Mg and Al-ion insertion in vanadium pentoxides and vanadium dioxides. RSC Advances, 2017, 7, 18643-18649.	1.7	66
26	Photofragment image analysis using the Onion-Peeling Algorithm. Computer Physics Communications, 2003, 154, 76-87.	3.0	63
27	Explicitly correlated MRCI-F12 potential energy surfaces for methane fit with several permutation invariant schemes and full-dimensional vibrational calculations. Molecular Physics, 2015, 113, 1823-1833.	0.8	63
28	Boosting inverted perovskite solar cell performance by using 9,9-bis(4-diphenylaminophenyl)fluorene functionalized with triphenylamine as a dopant-free hole transporting material. Journal of Materials Chemistry A, 2019, 7, 12507-12517.	5.2	62
29	One step facile synthesis of a novel anthanthrone dye-based, dopant-free hole transporting material for efficient and stable perovskite solar cells. Journal of Materials Chemistry C, 2018, 6, 3699-3708.	2.7	61
30	Controlled Redox of Lithium-Ion Endohedral Fullerene for Efficient and Stable Metal Electrode-Free Perovskite Solar Cells. Journal of the American Chemical Society, 2019, 141, 16553-16558.	6.6	61
31	Amorphous (Glassy) Carbon, a Promising Material for Sodium Ion Battery Anodes: a Combined First-Principles and Experimental Study. Journal of Physical Chemistry C, 2015, 119, 13496-13501.	1.5	60
32	Lowâ€Cost Alternative Highâ€Performance Holeâ€Transport Material for Perovskite Solar Cells and Its Comparative Study with Conventional SPIROâ€OMeTAD. Advanced Electronic Materials, 2017, 3, 1700139.	2.6	60
33	Aluminum doping improves the energetics of lithium, sodium, and magnesium storage in silicon: A first-principles study. Journal of Power Sources, 2015, 274, 65-70.	4.0	59
34	Thienylvinylenethienyl and Naphthalene Core Substituted with Triphenylaminesâ€"Highly Efficient Hole Transporting Materials and Their Comparative Study for Inverted Perovskite Solar Cells. Solar Rrl, 2017, 1, 1700105.	3.1	59
35	Machine learning for the solution of the SchrÃ¶dinger equation. Machine Learning: Science and Technology, 2020, 1, 013002.	2.4	58
36	Molecular Engineering Strategy for High Efficiency Fullerene-Free Organic Solar Cells Using Conjugated 1,8-Naphthalimide and Fluorenone Building Blocks. ACS Applied Materials & Interfaces, 2017, 9, 16967-16976.	4.0	56

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37	Comparative computational study of the diffusion of Li, Na, and Mg in silicon including the effect of vibrations. Solid State Ionics, 2013, 253, 157-163.	1.3	51
38	Exploring the sodium storage mechanism in disodium terephthalate as anode for organic battery using density-functional theory calculations. Journal of Power Sources, 2016, 324, 572-581.	4.0	51
39	Fitting sparse multidimensional data with low-dimensional terms. Computer Physics Communications, 2009, 180, 2002-2012.	3.0	50
40	Acene-based organic semiconductors for organic light-emitting diodes and perovskite solar cells. Journal of Materials Chemistry C, 2018, 6, 9017-9029.	2.7	50
41	Kinetic energy densities based on the fourth order gradient expansion: performance in different classes of materials and improvementviamachine learning. Physical Chemistry Chemical Physics, 2019, 21, 378-395.	1.3	46
42	Tuning the Charge Carrier Polarity of Organic Transistors by Varying the Electron Affinity of the Flanked Units in Diketopyrrolopyrroleâ€Based Copolymers. Advanced Functional Materials, 2020, 30, 1907452.	7.8	45
43	Polyaromatic Nanotweezers on Semiconducting Carbon Nanotubes for the Growth and Interfacing of Lead Halide Perovskite Crystal Grains in Solar Cells. Chemistry of Materials, 2020, 32, 5125-5133.	3.2	45
44	Highly Selective and Scalable Fullerene-Cation-Mediated Synthesis Accessing Cyclo[60]fullerenes with Five-Membered Carbon Ring and Their Application to Perovskite Solar Cells. Chemistry of Materials, 2019, 31, 8432-8439.	3.2	44
45	A model for the dissociative adsorption of N2O on Cu(100) using a continuous potential energy surface. Surface Science, 2010, 604, 555-561.	0.8	43
46	Synergistic Use of Pyridine and Selenophene in a Diketopyrrolopyrroleâ€Based Conjugated Polymer Enhances the Electron Mobility in Organic Transistors. Advanced Functional Materials, 2020, 30, 2000489.	7.8	43
47	Superior Noise Suppression, Response Time, and Device Stability of Nonâ€Fullerene System over Fullerene Counterpart in Organic Photodiode. Advanced Functional Materials, 2020, 30, 2001402.	7.8	42
48	A Density Functional Tight Binding Study of Acetic Acid Adsorption on Crystalline and Amorphous Surfaces of Titania. Molecules, 2015, 20, 3371-3388.	1.7	40
49	Charge and Discharge Processes and Sodium Storage in Disodium Pyridineâ€2,5â€Dicarboxylate Anodeâ€"Insights from Experiments and Theory. Advanced Energy Materials, 2018, 8, 1701572.	10.2	40
50	Superexcited state reconstruction of HCl using photoelectron and photoion imaging. Journal of Chemical Physics, 2004, 120, 767-777.	1.2	38
51	Ab initio study of Li, Mg and Al insertion into rutile VO₂: fast diffusion and enhanced voltages for multivalent batteries. Physical Chemistry Chemical Physics, 2017, 19, 22538-22545.	1.3	38
52	A comparative computational study of lithium and sodium insertion into van der Waals and covalent tetracyanoethylene (TCNE)-based crystals as promising materials for organic lithium and sodium ion batteries. Physical Chemistry Chemical Physics, 2016, 18, 8874-8880.	1.3	37
53	Dual chemosensor for the rapid detection of mercury(ii) pollution and biothiols. Analyst, The, 2019, 144, 4908-4916.	1.7	36
54	A benzothiadiazole end capped donorâ€"acceptor based small molecule for organic electronics. Physical Chemistry Chemical Physics, 2013, 15, 17064.	1.3	34

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55	Lithium and sodium storage on tetracyanoethylene (TCNE) and TCNE-(doped)-graphene complexes: A computational study. Materials Chemistry and Physics, 2015, 156, 180-187.	2.0	34
56	Computational dye design by changing the conjugation order: Failure of LR-TDDFT to predict relative excitation energies in organic dyes differing by the position of the methine unit. Chemical Physics Letters, 2012, 527, 51-56.	1.2	33
57	Voltage and capacity control of polyaniline based organic cathodes: An ab initio study. Journal of Power Sources, 2016, 336, 126-131.	4.0	33
58	Aluminium and magnesium insertion in sulfur-based spinels: a first-principles study. Physical Chemistry Chemical Physics, 2017, 19, 6076-6081.	1.3	33
59	Using an internal coordinate Gaussian basis and a space-fixed Cartesian coordinate kinetic energy operator to compute a vibrational spectrum with rectangular collocation. Journal of Chemical Physics, 2016, 145, 224110.	1.2	32
60	A computational study of lithium interaction with tetracyanoethylene (TCNE) and tetracyaniquinodimethane (TCNQ) molecules. Physical Chemistry Chemical Physics, 2016, 18, 1470-1477.	1.3	32
61	Random Sampling High Dimensional Model Representation Gaussian Process Regression (RS-HDMR-GPR) for Multivariate Function Representation: Application to Molecular Potential Energy Surfaces. Journal of Physical Chemistry A, 2020, 124, 7598-7607.	1.1	32
62	A model for recombination in Type II dye-sensitized solar cells: Catecholâ€“thiophene dyes. Chemical Physics Letters, 2011, 504, 230-235.	1.2	31
63	Photodissociation of hydrogen iodide in the A-band region 273â€“288 nm. Journal of Chemical Physics, 2002, 117, 9347-9352.	1.2	30
64	Computing the Anharmonic Vibrational Spectrum of UF₆ in 15 Dimensions with an Optimized Basis Set and Rectangular Collocation. Journal of Physical Chemistry A, 2015, 119, 9557-9567.	1.1	30
65	Naphthalimide end capped anthraquinone based solution-processable n-channel organic semiconductors: effect of alkyl chain engineering on charge transport. Journal of Materials Chemistry C, 2018, 6, 3774-3786.	2.7	30
66	1 potential, 2 potentials, 3 potentialsâ€“4: Untangling the UV photodissociation spectra of HI and DI. Journal of Chemical Physics, 2002, 117, 9353-9369.	1.2	29
67	On the advantages of a rectangular matrix collocation equation for computing vibrational spectra from small basis sets. Chemical Physics Letters, 2011, 511, 434-439.	1.2	29
68	High-Mobility Ambipolar Organic Thin-Film Transistor Processed From a Nonchlorinated Solvent. ACS Applied Materials & Interfaces, 2016, 8, 24325-24330.	4.0	29
69	Naphthalene flanked diketopyrrolopyrrole based organic semiconductors for high performance organic field effect transistors. New Journal of Chemistry, 2018, 42, 12374-12385.	1.4	29
70	Using a neural network based method to solve the vibrational SchrÃ¶dinger equation for H2O. Chemical Physics Letters, 2009, 474, 217-221.	1.2	27
71	Understanding the difference in cohesive energies between alpha and beta tin in DFT calculations. AIP Advances, 2016, 6, .	0.6	27
72	Doping of active electrode materials for electrochemical batteries: an electronic structure perspective. MRS Communications, 2017, 7, 523-540.	0.8	27

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73	Micromachining of ferrous metal with an ion implanted diamond cutting tool. Carbon, 2019, 152, 598-608.	5.4	27
74	Data-driven kinetic energy density fitting for orbital-free DFT: Linear vs Gaussian process regression. Journal of Chemical Physics, 2020, 153, 074104.	1.2	27
75	Polyaniline and CN-functionalized polyaniline as organic cathodes for lithium and sodium ion batteries: a combined molecular dynamics and density functional tight binding study in solid state. Physical Chemistry Chemical Physics, 2018, 20, 232-237.	1.3	27
76	Revisiting Ï€ backbonding: the influence of d orbitals on metalâ€“CO bonds and ligand red shifts. Physical Chemistry Chemical Physics, 2019, 21, 20814-20821.	1.3	26
77	Na-rich layered Na2Ti1â^'xCrxO3â^'x/2 (xâ€‰=â€‰0, 0.06): Na-ion battery cathode materials with high capacity and long cycle life. Scientific Reports, 2017, 7, 373.	1.6	25
78	A multimode-like scheme for selecting the centers of Gaussian basis functions when computing vibrational spectra. Chemical Physics, 2018, 509, 139-144.	0.9	25
79	Anharmonic vibrations of the carboxyl group in acetic acid on TiO2: implications for adsorption mode assignment in dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2013, 15, 10028.	1.3	24
80	Comparative density functional theory and density functional tight binding study of arginine and arginine-rich cell penetrating peptide TAT adsorption on anatase TiO₂. Physical Chemistry Chemical Physics, 2016, 18, 19902-19917.	1.3	24
81	Calculating anharmonic vibrational frequencies of molecules adsorbed on surfaces directly from ab initio energies with a molecule-independent method: H2O on Pt(111). Surface Science, 2011, 605, 616-622.	0.8	23
82	Comparative density functional theoryâ€“density functional tight binding study of fullerene derivatives: effects due to fullerene size, addends, and crystallinity on band structure, charge transport and optical properties. Physical Chemistry Chemical Physics, 2017, 19, 28330-28343.	1.3	23
83	Diketopyrrolopyrrole copolymers based chemical sensors for the detection and discrimination of volatile organic compounds. Sensors and Actuators B: Chemical, 2017, 251, 49-56.	4.0	22
84	Derivative coupling constants of NK1, NK7 dyes and their relation to excited state dynamics in solar cell applications. Chemical Physics Letters, 2011, 501, 580-586.	1.2	21
85	Parameterized Bases for Calculating Vibrational Spectra Directly from ab Initio Data Using Rectangular Collocation. Journal of Chemical Theory and Computation, 2012, 8, 2053-2061.	2.3	21
86	Computational study of interfacial charge transfer complexes of 2-anthroic acid adsorbed on a titania nanocluster for direct injection solar cells. Chemical Physics Letters, 2016, 660, 69-75.	1.2	21
87	Understanding doping strategies in the design of organic electrode materials for Li and Na ion batteries: an electronic structure perspective. Physical Chemistry Chemical Physics, 2017, 19, 13195-13209.	1.3	21
88	Diketopyrrolopyrrole-Based Dual-Acceptor Copolymers to Realize Tunable Charge Carrier Polarity of Organic Field-Effect Transistors and High-Performance Nonvolatile Ambipolar Flash Memories. ACS Applied Electronic Materials, 2020, 2, 1609-1618.	2.0	21
89	Two-photon state selection and angular momentum polarization probed by velocity map imaging: Application to H atom photofragment angular distributions from the photodissociation of two-photon state selected HCl and HBr. Journal of Chemical Physics, 2004, 121, 11802-11809.	1.2	20
90	A first-principles study of potassium insertion in crystalline vanadium oxide phases as possible potassium-ion battery cathode materials. MRS Communications, 2017, 7, 819-825.	0.8	20

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91	Triethylene Glycol Substituted Diketopyrrolopyrroleâ€•and Isoindigoâ€Dye Based Donorâ€“Acceptor Copolymers for Organic Lightâ€Emitting Electrochemical Cells and Transistors. Advanced Electronic Materials, 2020, 6, 1901414.	2.6	20
92	Comparison of alpha and beta tin for lithium, sodium, and magnesium storage: Anab initiostudy including phonon contributions. Journal of Chemical Physics, 2015, 143, 204701.	1.2	19
93	9-Fluorenone and 9,10-anthraquinone potential fused aromatic building blocks to synthesize electron acceptors for organic solar cells. New Journal of Chemistry, 2017, 41, 2899-2909.	1.4	19
94	Diketopyrrolopyrrole based organic semiconductors with different numbers of thiophene units: symmetry tuning effect on electronic devices. New Journal of Chemistry, 2018, 42, 4017-4028.	1.4	19
95	Intramolecular mode coupling of the isotopomers of water: a non-scalar charge density-derived perspective. Physical Chemistry Chemical Physics, 2020, 22, 2509-2520.	1.3	19
96	The effect of ligand substitution and water co-adsorption on the adsorption dynamics and energy level matching of amino-phenyl acid dyes on TiO2. Physical Chemistry Chemical Physics, 2012, 14, 1749-1755.	1.3	18
97	Communication: Favorable dimensionality scaling of rectangular collocation with adaptable basis functions up to 7 dimensions. Journal of Chemical Physics, 2013, 139, 051101.	1.2	18
98	Short Alkyl Chain Engineering Modulation on Naphthalene Flanked Diketopyrrolopyrrole toward Highâ€Performance Single Crystal Transistors and Organic Thin Film Displays. Advanced Electronic Materials, 2021, 7, 2000804.	2.6	18
99	A first-principles comparative study of lithium, sodium, and magnesium storage in pure and gallium-doped germanium: Competition between interstitial and substitutional sites. Journal of Chemical Physics, 2017, 146, 034706.	1.2	17
100	Random Sampling High Dimensional Model Representation Gaussian Process Regression (RS-HDMR-GPR) for representing multidimensional functions with machine-learned lower-dimensional terms allowing insight with a general method. Computer Physics Communications, 2022, 271, 108220.	3.0	17
101	Applying a Smolyak collocation method to Cl₂CO. Molecular Physics, 2017, 115, 1775-1785.	0.8	16
102	High-Working-Pressure Sputtering of ZnO for Stable and Efficient Perovskite Solar Cells. ACS Applied Electronic Materials, 2019, 1, 389-396.	2.0	16
103	Curvature drastically changes diffusion properties of Li and Na on graphene. MRS Communications, 2013, 3, 171-175.	0.8	15
104	On the Choice of the Discount Rate and the Role of Financial Variables and Physical Parameters in Estimating the Levelized Cost of Energy. International Journal of Financial Studies, 2013, 1, 54-61.	1.1	15
105	Highly accurate local pseudopotentials of Li, Na, and Mg for orbital free density functional theory. Chemical Physics Letters, 2015, 622, 99-103.	1.2	15
106	A triphenylamine substituted quinacridone derivative for solution processed organic light emitting diodes. Materials Chemistry and Physics, 2018, 206, 56-63.	2.0	15
107	Naphthalimide end-capped diphenylacetylene: a versatile organic semiconductor for blue light emitting diodes and a donor or an acceptor for solar cells. New Journal of Chemistry, 2019, 43, 9243-9254.	1.4	15
108	Three-body interactions in clusters COâ€“(pH2)n. Chemical Physics Letters, 2010, 493, 229-233.	1.2	14

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109	A Study of Diphenylfumaronitrile and Furanâ€Substituted Diketopyrrolopyrrole Alternating Copolymer and Its Thinâ€Film Transistors. Macromolecular Chemistry and Physics, 2014, 215, 725-732.	1.1	14
110	Comparative density functional theory and density functional tight binding study of 2-anthroic acid on TiO2. Chemical Physics Letters, 2016, 643, 16-20.	1.2	14
111	A comparative study of electrochemical, optical properties and electropolymerization behavior of thiophene- and furan-substituted diketopyrrolopyrrole. Journal of Materials Research, 2017, 32, 810-821.	1.2	14
112	First-Principle Insights Into Molecular Design for High-Voltage Organic Electrode Materials for Mg Based Batteries. Frontiers in Chemistry, 2020, 8, 83.	1.8	14
113	Exploration of the forbidden regions of the Ramachandran plot (Ï•-Ï^) with QTAIM. Physical Chemistry Chemical Physics, 2017, 19, 26423-26434.	1.3	13
114	Experimental and Theoretical Studies of Trisodiumâ€1,3,5â€Benzene Tricarboxylate as a Lowâ€Voltage Anode Material for Sodiumâ€Ion Batteries. Energy Technology, 2019, 7, 1801030.	1.8	13
115	CONUNDrum: A program for orbital-free density functional theory calculations. Computer Physics Communications, 2020, 256, 107365.	3.0	13
116	Easy representation of multivariate functions with low-dimensional terms via Gaussian process regression kernel design: applications to machine learning of potential energy surfaces and kinetic energy densities from sparse data. Machine Learning: Science and Technology, 2022, 3, 01LT02.	2.4	13
117	Machine Learning Optimization of the Collocation Point Set for Solving the Kohnâ€“Sham Equation. Journal of Physical Chemistry A, 2019, 123, 10631-10642.	1.1	12
118	Organic electrode materials for lithium and post-lithium batteries: an ab initio perspective on design. Current Opinion in Green and Sustainable Chemistry, 2019, 17, 8-14.	3.2	12
119	One-step direct oxidation of fullerene-fused alkoxy ethers to ketones for evaporable fullerene derivatives. Communications Chemistry, 2021, 4, .	2.0	12
120	Materials Design and Optimization for Next-Generation Solar Cell and Light-Emitting Technologies. Journal of Physical Chemistry Letters, 2021, 12, 4638-4657.	2.1	12
121	Computational vibrational spectroscopy of moleculeâ€“surface interactions: what is still difficult and what can be done about it. Physical Chemistry Chemical Physics, 2022, 24, 15158-15172.	1.3	12
122	Photofragment image analysis via pattern recognition. Review of Scientific Instruments, 2004, 75, 2435-2445.	0.6	11
123	Nonspectral Methods for Solving the SchrÃ¶dinger Equation for Electronic and Vibrational Problems. Journal of Physical Chemistry Letters, 2011, 2, 2193-2199.	2.1	11
124	Towards Accurate Spectroscopic Identification of Species at Catalytic Surfaces: Anharmonic Vibrations of Formate on AuPt. Materials Research Society Symposia Proceedings, 2012, 1484, 1.	0.1	11
125	Effect of nuclear vibrations, temperature, co-adsorbed water, and dye orientation on light absorption, charge injection and recombination conditions in organic dyes on TiO₂. Physical Chemistry Chemical Physics, 2013, 15, 1141-1147.	1.3	11
126	Quantifying the Distribution of the Stoichiometric Composition of Anticancer Peptide Lycosin-I on the Lipid Membrane with Single Molecule Spectroscopy. Journal of Physical Chemistry B, 2016, 120, 3081-3088.	1.2	11

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127	Using rectangular collocation with finite difference derivatives to solve electronic SchrÃ¶dinger equation. Journal of Chemical Physics, 2018, 149, 204105.	1.2	11
128	Significant Improvement of Optoelectronic and Photovoltaic Properties by Incorporating Thiophene in a Solution-Processable Dâ€“Aâ€“D Modular Chromophore. Molecules, 2015, 20, 21787-21801.	1.7	10
129	Orbital order switching in molecular calculations using GGA functionals: Qualitative errors in materials modeling for electrochemical power sources and how to fix them. Chemical Physics Letters, 2016, 659, 270-276.	1.2	10
130	Insertion of Mono- vs. Bi- vs. Trivalent Atoms in Prospective Active Electrode Materials for Electrochemical Batteries: An ab Initio Perspective. Energies, 2017, 10, 2061.	1.6	10
131	Influence of the aggregate state on band structure and optical properties of C60 computed with different methods. Journal of Chemical Physics, 2018, 148, 204301.	1.2	10
132	Comparison of optical absorption spectra of organic molecules and aggregates computed from real frequency dependent polarizability to TD-DFT and the dipole approximation. Journal of Chemical Physics, 2018, 149, 044114.	1.2	10
133	Phthalimide and naphthalimide: Effect of end-capping groups on molecular properties and photovoltaic performance of 9-fluorenone based acceptors for organic solar cells. Organic Electronics, 2018, 62, 12-20.	1.4	10
134	Indenofluorene-based-copolymers: Influence of electron-deficient benzothiadiazole (BT) and benzooxadiazole (BO) moieties on light emitting devices. Organic Electronics, 2019, 70, 14-24.	1.4	10
135	Effect of organic cation states on electronic properties of mixed organicâ€“inorganic halide perovskite clusters. Physical Chemistry Chemical Physics, 2019, 21, 8161-8169.	1.3	10
136	Fluorination of pyrene-based organic semiconductors enhances the performance of light emitting diodes and halide perovskite solar cells. Organic Electronics, 2020, 77, 105524.	1.4	10
137	Nonparametric Local Pseudopotentials with Machine Learning: A Tin Pseudopotential Built Using Gaussian Process Regression. Journal of Physical Chemistry A, 2020, 124, 11111-11124.	1.1	10
138	Directional Carrier Polarity Tunability in Ambipolar Organic Transistors Based on Diketopyrrolopyrrole and Bithiophene Imide Dual-Acceptor Semiconducting Polymers. Chemistry of Materials, 2022, 34, 3140-3151.	3.2	10
139	Computational design of small organic dyes with strong visible absorption by controlled quinoidization of the thiophene unit. Chemical Physics Letters, 2014, 593, 14-19.	1.2	9
140	Disodium Pyridine Dicarboxylate vs Disodium Terephthalate as Anode Materials for Organic Na Ion Batteries: Effect of Molecular Structure on Voltage from the Molecular Modeling Perspective. MRS Advances, 2017, 2, 3231-3235.	0.5	9
141	A new pyrene cored small organic molecule with a flexible alkyl spacer: a potential solution processable blue emitter with bright photoluminescence. New Journal of Chemistry, 2017, 41, 11383-11390.	1.4	9
142	Inverse Multiquadratic Functions as the Basis for the Rectangular Collocation Method to Solve the Vibrational SchrÃ¶dinger Equation. Mathematics, 2018, 6, 253.	1.1	9
143	Lithium Attachment to C60 and Nitrogen- and Boron-Doped C60: A Mechanistic Study. Materials, 2019, 12, 2136.	1.3	9
144	Naphthalene flanked diketopyrrolopyrrole: A new DPP family member and its comparative optoelectronic properties with thiophene- and furan- flanked DPP counterparts. Organic Electronics, 2019, 74, 290-298.	1.4	9

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145	A Scheme for Ultrasensitive Detection of Molecules with Vibrational Spectroscopy in Combination with Signal Processing. Molecules, 2019, 24, 776.	1.7	9
146	Effect of Nuclear Motion on Charge Transport in Fullerenes: A Combined Density Functional Tight Bindingâ€"Density Functional Theory Investigation. Frontiers in Energy Research, 2019, 7, .	1.2	9
147	Ab initio modeling and design of vanadia-based electrode materials for post-lithium batteries. Journal Physics D: Applied Physics, 2020, 53, 083001.	1.3	9
148	Versatile nature of anthanthrone based polymers as active multifunctional semiconductors for various organic electronic devices. Materials Advances, 2020, 1, 3428-3438.	2.6	9
149	Theoretical analysis of the solvatochromism of organic dyes differing by the conjugation sequence. Journal of Photonics for Energy, 2012, 2, 028001.	0.8	8
150	A computational study of adsorption and vibrations of UF6 on graphene derivatives: Conditions for 2D enrichment. Carbon, 2015, 81, 800-806.	5.4	8
151	Defects in crystalline PVDF: a density functional theory-density functional tight binding study. Physical Chemistry Chemical Physics, 2017, 19, 7560-7567.	1.3	8
152	Investigation of thiophene flanked diketopyrrolopyrrole monomers with straight and branched alkyl chains and their electropolymerization study. Journal of Materials Research, 2017, 32, 2707-2718.	1.2	8
153	Solvation-Free Li⁺ Lewis Acid Enhancing Reaction: Kinetic Study of [5,6]-Li⁺@PCBM to [6,6]-Li⁺@PCBM. Organic Letters, 2020, 22, 7239-7243.	2.4	8
154	Modeling of plasmonic properties of nanostructures for next generation solar cells and beyond. Advances in Physics: X, 2021, 6, .	1.5	8
155	Advanced Machine Learning Methods for Learning from Sparse Data in High-Dimensional Spaces: A Perspective on Uses in the Upstream of Development of Novel Energy Technologies. Physchem, 2022, 2, 72-95.	0.5	8
156	Computational design of new organics dyes with improved solar absorbance for dye-sensitized solar cells. MRS Communications, 2013, 3, 37-39.	0.8	7
157	Shear-induced conformation change in Î±-crystalline nylon6. Applied Physics Letters, 2014, 105, .	1.5	7
158	A Comparative Computational Study of Li, Na, and Mg Insertion in Î±-Sn. Materials Research Society Symposia Proceedings, 2014, 1678, 1.	0.1	7
159	A comparative computational study of the diffusion of Na and Li atoms in Sn(111) nanosheets. Solid State Ionics, 2014, 268, 273-276.	1.3	7
160	Addition to â€œOn the Charge State of Titanium in Titanium Dioxideâ€• Journal of Physical Chemistry Letters, 2017, 8, 3945-3946.	2.1	7
161	The role of weak interactions in characterizing peptide folding preferences using a QTAIM interpretation of the Ramachandran plot (Ï•â€Ï). International Journal of Quantum Chemistry, 2018, 118, e25456.	1.0	7
162	The role of solvent charge donation in the stabilization of metal ions in aqueous solution. MRS Communications, 2018, 8, 1139-1144.	0.8	7

#	Article	IF	Citations
163	Theoretical study of the origin of the large difference in the visible absorption spectra of organic dyes containing a thienylmethine unit and differing by the methine unit position. , 2011, , .		6
164	Effects of Nuclear Vibrations on the Energetics of Polythiophene: Quantized Energy Molecular Dynamics. Australian Journal of Chemistry, 2013, 66, 1021.	0.5	6
165	Bridging the Fields of Solar Cell and Battery Research to Develop High-Performance Anodes for Photoelectrochemical Cells and Metal Ion Batteries. Challenges, 2013, 4, 116-135.	0.9	6
166	Defects in alpha and gamma crystalline nylon6: A computational study. AIP Advances, 2015, 5, 107123.	0.6	6
167	A Comparative Density Functional Theory and Density Functional Tight Binding Study of Phases of Nitrogen Including a High Energy Density Material N8. Computation, 2015, 3, 574-585.	1.0	6
168	Sodium Interaction with Disodium Terephthalate Molecule: an Ab Initio Study. MRS Advances, 2016, 1, 3579-3584.	0.5	6
169	A Comparative First-Principles Study of Lithium, Sodium and Magnesium Insertion Energetics in Brookite Titanium Dioxide. MRS Advances, 2019, 4, 837-842.	0.5	6
170	Interstitial versus substitutional metal insertion in V2O5 as post-lithium ion battery cathode: a comparative GGA/GGA + U study with localized bases. MRS Communications, 2020, 10, 259-264.	0.8	6
171	Reply to the â€˜Comment on â€œRevisiting Ï€ backbonding: the influence of d orbitals on metalâ€“CO bonds and ligand red shiftsâ€â€™ by G. Frenking and S. Pan, Phys. Chem. Chem. Phys., 2019, 22, DOI: 10.1039/C9CP05951B. Physical Chemistry Chemical Physics, 2020, 22, 5380-5382.	1.3	6
172	Naphthalene Flanked Diketopyrrolopyrrole: A New Functional Dye Based Optical Sensors for Monitoring Cyanide Ions in Water. Advanced Materials Technologies, 0, , 2100170.	3.0	6
173	Effect of nuclear vibrations, temperature, and orientation on injection and recombination conditions in amino-phenyl acid dyes on TiO 2. Proceedings of SPIE, 2012, , .	0.8	5
174	Theoretical analysis of the absorption spectra of organic dyes differing by the conjugation sequence: illusion of negative solvatochromism. , 2012, , .		5
175	Isotopic Substitution as a Strategy to Control Non-Adiabatic Dynamics in Photoelectrochemical Cells: Surface Complexes between TiO$_{2}$ and Dicyanomethylene Compounds. Japanese Journal of Applied Physics, 2012, 51, 10NE03.	0.8	5
176	Li Storage on TCNE and TCNE-(Doped)-Graphene Complexes: a Computational Study. Materials Research Society Symposia Proceedings, 2014, 1679, 1.	0.1	5
177	Pyrrolo[3,2-b]pyrrole-1,4-dione (IsoDPP) End Capped with Napthalimide or Phthalimide: Novel Small Molecular Acceptors for Organic Solar Cells. Molecules, 2020, 25, 4700.	1.7	5
178	Extracting Functional Dependence from Sparse Data Using Dimensionality Reduction: Application to Potential Energy Surface Construction. Lecture Notes in Computational Science and Engineering, 2011, , 133-149.	0.1	5
179	Configuration of ring-down spectrometers for maximum sensitivity. Canadian Journal of Chemistry, 2004, 82, 873-879.	0.6	4
180	Effect of Isotopic Substitution on Elementary Processes in Dye-Sensitized Solar Cells: Deuterated Amino-Phenyl Acid Dyes on TiO2. Computation, 2013, 1, 1-15.	1.0	4

#	Article	IF	Citations
181	Computational design of small phenothiazine dyes for dye-sensitized solar cells by functionalizations affecting the thiophene unit. Journal of Molecular Modeling, 2015, 21, 67.	0.8	4
182	Dopantâ€“dopant interactions in beryllium doped indium gallium arsenide: An ab initio study. Journal of Materials Research, 2018, 33, 401-413.	1.2	4
183	First-Principles Study of the Calcium Insertion in Layered and Non-Layered Phases of Vanadia. MRS Advances, 2018, 3, 3507-3512.	0.5	4
184	Aggregate-State Effects in the Atomistic Modeling of Organic Materials for Electrochemical Energy Conversion and Storage Devices: A Perspective. Molecules, 2020, 25, 2233.	1.7	4
185	Electrochemical Performance of Bâ€Type Vanadium Dioxide as a Sodiumâ€ion Battery Cathode: A Combined Experimental and Theoretical Study. ChemElectroChem, 2020, 7, 3151-3159.	1.7	4
186	Structural Geometry Variation of 1,4-Naphthalene-Based Co-Polymers to Tune the Device Performance of PVK-Host-Based OLEDs. Polymers, 2021, 13, 2914.	2.0	4
187	Isotopic Substitution as a Strategy to Control Non-Adiabatic Dynamics in Photoelectrochemical Cells: Surface Complexes between TiO2and Dicyanomethylene Compounds. Japanese Journal of Applied Physics, 2012, 51, 10NE03.	0.8	4
188	Computational study of Mg insertion into amorphous silicon: advantageous energetics over crystalline silicon for Mg storage. Materials Research Society Symposia Proceedings, 2013, 1540, 3601.	0.1	3
189	Achieving Improved Solar Absorbance of Small Organic Dyes Featuring Quinoidized Five-Membered Heterocycles. Materials Research Society Symposia Proceedings, 2014, 1667, 26.	0.1	3
190	Mg and K Insertion in Glassy Amorphous Carbon vs Graphite as Potential Anode Materials: an Ab Initio Study. MRS Advances, 2016, 1, 3069-3074.	0.5	3
191	Grown-in beryllium diffusion in indium gallium arsenide: An ab initio, continuum theory and kinetic Monte Carlo study. Acta Materialia, 2017, 125, 455-464.	3.8	3
192	A Model for Estimating Chemical Potentials in Ternary Semiconductor Compounds: the Case of InGaAs. MRS Advances, 2017, 2, 2909-2914.	0.5	3
193	The Role of Local DFT+U Minima in the First-Principles Modeling of the Metalâ€“Insulator Transition in Vanadium Dioxide. Journal of Physical Chemistry A, 2022, 126, 3604-3611.	1.1	3
194	Effect of the adsorption of ethylene carbonate on Si surfaces on the Li insertion behavior. Chemical Physics Letters, 2013, 585, 157-161.	1.2	2
195	Role of Inter-Dopant Interactions on the Diffusion of Li and Na Atoms in Bulk Si Anodes. Materials Research Society Symposia Proceedings, 2013, 1541, 75601.	0.1	2
196	Oxygen Redox Activity in Cathodes: A Common Phenomenon Calling for Density-Based Descriptors. Journal of Physical Chemistry C, 2020, 124, 19962-19968.	1.5	2
197	Can doping of transition metal oxide cathode materials increase achievable voltages with multivalent metals?. International Journal of Quantum Chemistry, 2021, 121, e26439.	1.0	2
198	Density-Based Descriptors of Redox Reactions Involving Transition Metal Compounds as a Reality-Anchored Framework: A Perspective. Molecules, 2021, 26, 5541.	1.7	2

#	Article	IF	Citations
199	Reflections of a Computer Poet on American Social Dynamics (Or How This Makes Sense). Advances in Literary Study, 2014, 02, 47-57.	0.0	2
200	Carbon/air secondary battery system and demonstration of its charge-discharge. Journal of Power Sources, 2021, 516, 230681.	4.0	2
201	Theoretical Insight Into Diamond Doping and Its Possible Effect on Diamond Tool Wear During Cutting of Steel. Frontiers in Materials, 2021, 8, .	1.2	2
202	Effect of Surface Treatment on the Mode I Debonding of Interface Between Silica and Nylon6. MRS Advances, 2016, 1, 2717-2722.	0.5	1
203	First-Principles Study of the Electrochemical Sodiation of Rutile-Type Vanadium Dioxide. MRS Advances, 2020, 5, 1467-1474.	0.5	1
204	Effective passivation of TiO2/Si by interlayer SiOx controlled by scanning zone annealing for perovskite/Si tandem solar cell. Solar Energy, 2022, 236, 772-781.	2.9	1
205	Fluorenone and triphenylamine based donorâ€“acceptorâ€“donor (Dâ€“Aâ€“D) for solution-processed organic light-emitting diodes. Flexible and Printed Electronics, 2022, 7, 025009.	1.5	1
206	Representing potential energy surfaces with neural networks and high dimensional model representations. , 2012, , .		0
207	Adsorption of UF6on Graphene Derivatives: a Computational Study of Conditions for 2D Enrichment. Materials Research Society Symposia Proceedings, 2014, 1683, 32.	0.1	0
208	Preface to the IWCMM23 special issue. Computational Materials Science, 2014, 94, 1.	1.4	0
209	Adsorption and Light Absorption Properties of 2-Anthroic Acid on Titania: a Density Functional Theory â€" Time-Dependent Density Functional Theory Study. MRS Advances, 2016, 1, 2795-2800.	0.5	0
210	Special Issue â€œMolecular Engineering for Electrochemical Power Sourcesâ€• Molecules, 2016, 21, 1524.	1.7	0
211	PhysChem: A New Physical Chemistry Journal. Physchem, 2021, 1, 1-3.	0.5	0
212	Comparative AB Initio Study of Lithium Storage in Amorphous and Crystalline TiO 2. , 2014, , .		0
213	Li and Na Storage on TCNE:Computational Study. , 2014, , .		0
214	Conjugated 1,8-Naphthalimide Based Solution Processable n-Type Semiconductors for Organic Electronics. , 0, , .		0
215	Modeling Methods for Plasmonic Effects in Halide Perovskite Based Systems for Photonics Applications. , 2021, , 1-52.		0
216	Welcome to Physchem: Status and Prospects. Physchem, 2022, 2, 16-17.	0.5	0