Sergei Manzhos

List of Publications by Citations

203 papers	4,577 citations	38 h-index	57 g-index
224 ext. papers	5,387 ext. citations	5 avg, IF	6.44 L-index

#	Paper	IF	Citations
203	A random-sampling high dimensional model representation neural network for building potential energy surfaces. *Journal of Chemical Physics*, **2006**, 125, 084109	3.9	186
202	Neural network-based approaches for building high dimensional and quantum dynamics-friendly potential energy surfaces. *International Journal of Quantum Chemistry*, **2015**, 115, 1012-1020	2.1	140
201	A nested molecule-independent neural network approach for high-quality potential fits. *Journal of Physical Chemistry A*, **2006**, 110, 5295-304	2.8	140
200	Using neural networks to represent potential surfaces as sums of products. *Journal of Chemical Physics*, **2006**, 125, 194105	3.9	138
199	Organic interfacial materials for perovskite-based optoelectronic devices. *Energy and Environmental Science*, **2019**, 12, 1177-1209	35.4	125
198	Molecular Engineering Using an Anthanthrone Dye for Low-Cost Hole Transport Materials: A Strategy for Dopant-Free, High-Efficiency, and Stable Perovskite Solar Cells. *Advanced Energy Materials*, **2018**, 8, 1703007	21.8	115
197	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	3.9	96
196	Using neural networks, optimized coordinates, and high-dimensional model representations to obtain a vinyl bromide potential surface. *Journal of Chemical Physics*, **2008**, 129, 224104	3.9	88
195	Using redundant coordinates to represent potential energy surfaces with lower-dimensional functions. *Journal of Chemical Physics*, **2007**, 127, 014103	3.9	87
194	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	8.9	85
193	Phenothiazine and carbazole substituted pyrene based electroluminescent organic semiconductors for OLED devices. *Journal of Materials Chemistry C*, **2016**, 4, 1009-1018	7.1	78
192	A Comparative Computational Study of Structures, Diffusion, and Dopant Interactions between Li and Na Insertion into Si. *Applied Physics Express*, **2013**, 6, 027301	2.4	71
191	A computational study of Na behavior on graphene. *Applied Surface Science*, **2015**, 333, 235-243	6.7	71
190	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	8.9	69
189	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	3.8	69
188	A computational study of the insertion of Li, Na, and Mg atoms into Si(111) nanosheets. *Nano Energy*, **2013**, 2, 1149-1157	17.1	68
187	Neural Network Potential Energy Surfaces for Small Molecules and Reactions. *Chemical Reviews*, **2021**, 121, 10187-10217	68.1	63

186	Controlling Na diffusion by rational design of Si-based layered architectures. *Physical Chemistry Chemical Physics*, **2014**, 16, 4260-7	3.6	62
185	Photofragment image analysis using the Onion-Peeling Algorithm. *Computer Physics Communications*, **2003**, 154, 76-87	4.2	58
184	Comparative computational study of the energetics of Li, Na, and Mg storage in amorphous and crystalline silicon. *Computational Materials Science*, **2014**, 94, 214-217	3.2	56
183	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	11	55
182	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	13	52
181	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	1.7	52
180	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	8.9	50
179	On the Charge State of Titanium in Titanium Dioxide. *Journal of Physical Chemistry Letters*, **2017**, 8, 1593-1598	6.4	49
178	Thienylvinylenethienyl and Naphthalene Core Substituted with Triphenylamines: Highly Efficient Hole Transporting Materials and Their Comparative Study for Inverted Perovskite Solar Cells. *Solar Rrl*, **2017**, 1, 1700105	7.1	49
177	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	7.1	48
176	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	8.9	45
175	Achieving High Efficiency in Solution-Processed Perovskite Solar Cells Using C/C Mixed Fullerenes. *ACS Applied Materials & Interfaces*, **2018**, 10, 39590-39598	9.5	45
174	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	3.8	44
173	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	3.3	43
172	Low-Cost Alternative High-Performance Hole-Transport Material for Perovskite Solar Cells and Its Comparative Study with Conventional SPIRO-OMeTAD. *Advanced Electronic Materials*, **2017**, 3, 1700139	6.4	43
171	Fitting sparse multidimensional data with low-dimensional terms. *Computer Physics Communications*, **2009**, 180, 2002-2012	4.2	43
170	Comparison of Li, Na, Mg and Al-ion insertion in vanadium pentoxides and vanadium dioxides. *RSC Advances*, **2017**, 7, 18643-18649	3.7	42
169	Acene-based organic semiconductors for organic light-emitting diodes and perovskite solar cells. *Journal of Materials Chemistry C*, **2018**, 6, 9017-9029	7.1	41

168	A model for the dissociative adsorption of N2O on Cu(1 0 0) using a continuous potential energy surface. *Surface Science*, **2010**, 604, 555-561	1.8	39
167	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	9.5	38
166	Superexcited state reconstruction of HCl using photoelectron and photoion imaging. *Journal of Chemical Physics*, **2004**, 120, 767-77	3.9	38
165	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	16.4	35
164	All-Rounder Low-Cost Dopant-Free D-A-D Hole-Transporting Materials for Efficient Indoor and Outdoor Performance of Perovskite Solar Cells. *Advanced Electronic Materials*, **2020**, 6, 1900884	6.4	35
163	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, 8874-80	3.6	34
162	A density functional tight binding study of acetic acid adsorption on crystalline and amorphous surfaces of titania. *Molecules*, **2015**, 20, 3371-88	4.8	33
161	Machine learning for the solution of the Schr□dinger equation. *Machine Learning: Science and Technology*, **2020**, 1, 013002	5.1	32
160	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	2.5	32
159	Lithium and sodium storage on tetracyanoethylene (TCNE) and TCNE-(doped)-graphene complexes: A computational study. *Materials Chemistry and Physics*, **2015**, 156, 180-187	4.4	31
158	A benzothiadiazole end capped donor-acceptor based small molecule for organic electronics. *Physical Chemistry Chemical Physics*, **2013**, 15, 17064-9	3.6	30
157	Kinetic energy densities based on the fourth order gradient expansion: performance in different classes of materials and improvement via machine learning. *Physical Chemistry Chemical Physics*, **2018**, 21, 378-395	3.6	29
156	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	9.6	29
155	A model for recombination in Type II dye-sensitized solar cells: Catechol□hiophene dyes. *Chemical Physics Letters*, **2011**, 504, 230-235	2.5	29
154	Aluminium and magnesium insertion in sulfur-based spinels: a first-principles study. *Physical Chemistry Chemical Physics*, **2017**, 19, 6076-6081	3.6	28
153	A computational study of lithium interaction with tetracyanoethylene (TCNE) and tetracyaniquinodimethane (TCNQ) molecules. *Physical Chemistry Chemical Physics*, **2016**, 18, 1470-7	3.6	28
152	An improved neural network method for solving the Schr□dinger equation. *Canadian Journal of Chemistry*, **2009**, 87, 864-871	0.9	28
151	Charge and Discharge Processes and Sodium Storage in Disodium Pyridine-2,5-Dicarboxylate Anode□nsights from Experiments and Theory. *Advanced Energy Materials*, **2018**, 8, 1701572	21.8	28

150	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	9.6	27
149	Voltage and capacity control of polyaniline based organic cathodes: An ab initio study. *Journal of Power Sources*, **2016**, 336, 126-131	8.9	27
148	Using a neural network based method to solve the vibrational Schr□dinger equation for H2O. *Chemical Physics Letters*, **2009**, 474, 217-221	2.5	27
147	1 potential, 2 potentials, 3 potentials□: Untangling the UV photodissociation spectra of HI and DI. *Journal of Chemical Physics*, **2002**, 117, 9353-9369	3.9	27
146	Photodissociation of hydrogen iodide in the A-band region 273□88 nm. *Journal of Chemical Physics* , **2002**, 117, 9347-9352	3.9	27
145	Tuning the Charge Carrier Polarity of Organic Transistors by Varying the Electron Affinity of the Flanked Units in Diketopyrrolopyrrole-Based Copolymers. *Advanced Functional Materials*, **2020**, 30, 1907452	15.6	27
144	Dual chemosensor for the rapid detection of mercury(ii) pollution and biothiols. *Analyst, The*, **2019**, 144, 4908-4916	5	26
143	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	7.1	24
142	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	3.9	23
141	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, 9557-67	2.8	22
140	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, 10028-34	3.6	22
139	Ab initio study of Li, Mg and Al insertion into rutile VO: fast diffusion and enhanced voltages for multivalent batteries. *Physical Chemistry Chemical Physics*, **2017**, 19, 22538-22545	3.6	22
138	On the advantages of a rectangular matrix collocation equation for computing vibrational spectra from small basis sets. *Chemical Physics Letters*, **2011**, 511, 434-439	2.5	22
137	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	1.8	22
136	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*, **2017**, 20, 232-237	3.6	22
135	High-Mobility Ambipolar Organic Thin-Film Transistor Processed From a Nonchlorinated Solvent. *ACS Applied Materials & Interfaces*, **2016**, 8, 24325-30	9.5	22
134	Superior Noise Suppression, Response Time, and Device Stability of Non-Fullerene System over Fullerene Counterpart in Organic Photodiode. *Advanced Functional Materials*, **2020**, 30, 2001402	15.6	21
133	Comparative density functional theory-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	3.6	20

132	Synergistic Use of Pyridine and Selenophene in a Diketopyrrolopyrrole-Based Conjugated Polymer Enhances the Electron Mobility in Organic Transistors. *Advanced Functional Materials*, **2020**, 30, 2000489	15.6	20
131	Naphthalene flanked diketopyrrolopyrrole based organic semiconductors for high performance organic field effect transistors. *New Journal of Chemistry*, **2018**, 42, 12374-12385	3.6	20
130	Doping of active electrode materials for electrochemical batteries: an electronic structure perspective. *MRS Communications*, **2017**, 7, 523-540	2.7	20
129	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	2.5	20
128	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, 11802-9	3.9	20
127	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	2.5	20
126	Diketopyrrolopyrrole copolymers based chemical sensors for the detection and discrimination of volatile organic compounds. *Sensors and Actuators B: Chemical*, **2017**, 251, 49-56	8.5	19
125	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, 19902-17	3.6	19
124	Na-rich layered NaTiCrO (x = 0, 0.06): Na-ion battery cathode materials with high capacity and long cycle life. *Scientific Reports*, **2017**, 7, 373	4.9	18
123	Diketopyrrolopyrrole based organic semiconductors with different numbers of thiophene units: symmetry tuning effect on electronic devices. *New Journal of Chemistry*, **2018**, 42, 4017-4028	3.6	18
122	A multimode-like scheme for selecting the centers of Gaussian basis functions when computing vibrational spectra. *Chemical Physics*, **2018**, 509, 139-144	2.3	18
121	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	3.6	17
120	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	3.6	17
119	Revisiting π-backbonding: the influence of d orbitals on metal-CO bonds and ligand red shifts. *Physical Chemistry Chemical Physics*, **2019**, 21, 20814-20821	3.6	17
118	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, 1749-55	3.6	17
117	Parameterized Bases for Calculating Vibrational Spectra Directly from ab Initio Data Using Rectangular Collocation. *Journal of Chemical Theory and Computation*, **2012**, 8, 2053-61	6.4	16
116	Communication: favorable dimensionality scaling of rectangular collocation with adaptable basis functions up to 7 dimensions. *Journal of Chemical Physics*, **2013**, 139, 051101	3.9	16
115	Comparison of alpha and beta tin for lithium, sodium, and magnesium storage: An ab initio study including phonon contributions. *Journal of Chemical Physics*, **2015**, 143, 204701	3.9	15

114	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	2.8	15
113	Understanding the difference in cohesive energies between alpha and beta tin in DFT calculations. *AIP Advances*, **2016**, 6, 045116	1.5	15
112	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	3.9	14
111	Applying a Smolyak collocation method to Cl2CO. *Molecular Physics*, **2017**, 115, 1775-1785	1.7	13
110	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	2.7	13
109	A Study of Diphenylfumaronitrile and Furan-Substituted Diketopyrrolopyrrole Alternating Copolymer and Its Thin-Film Transistors. *Macromolecular Chemistry and Physics*, **2014**, 215, 725-732	2.6	13
108	High-Working-Pressure Sputtering of ZnO for Stable and Efficient Perovskite Solar Cells. *ACS Applied Electronic Materials*, **2019**, 1, 389-396	4	13
107	Curvature drastically changes diffusion properties of Li and Na on graphene. *MRS Communications*, **2013**, 3, 171-175	2.7	12
106	A triphenylamine substituted quinacridone derivative for solution processed organic light emitting diodes. *Materials Chemistry and Physics*, **2018**, 206, 56-63	4.4	12
105	Micromachining of ferrous metal with an ion implanted diamond cutting tool. *Carbon*, **2019**, 152, 598-608	10.4	11
104	Triethylene Glycol Substituted Diketopyrrolopyrrole- and Isoindigo-Dye Based Donor–Acceptor Copolymers for Organic Light-Emitting Electrochemical Cells and Transistors. *Advanced Electronic Materials*, **2020**, 6, 1901414	6.4	11
103	Comparative density functional theory and density functional tight binding study of 2-anthroic acid on TiO2. *Chemical Physics Letters*, **2016**, 643, 16-20	2.5	11
102	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, 1141-7	3.6	11
101	Exploration of the forbidden regions of the Ramachandran plot (?-) with QTAIM. *Physical Chemistry Chemical Physics*, **2017**, 19, 26423-26434	3.6	11
100	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	1.7	11
99	Three-body interactions in clusters CO(pH2)n. *Chemical Physics Letters*, **2010**, 493, 229-233	2.5	11
98	Data-driven kinetic energy density fitting for orbital-free DFT: Linear vs Gaussian process regression. *Journal of Chemical Physics*, **2020**, 153, 074104	3.9	11
97	Short Alkyl Chain Engineering Modulation on Naphthalene Flanked Diketopyrrolopyrrole toward High-Performance Single Crystal Transistors and Organic Thin Film Displays. *Advanced Electronic Materials*, **2021**, 7, 2000804	6.4	11

96	A comparative study of electrochemical, optical properties and electropolymerization behavior of thiophene- and furan-substituted diketopyrrolopyrrole. *Journal of Materials Research*, **2017**, 32, 810-821	2.5	10
95	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	2.5	10
94	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, 3081-8	3.4	10
93	Experimental and Theoretical Studies of Trisodium-1,3,5-Benzene Tricarboxylate as a Low-Voltage Anode Material for Sodium-Ion Batteries. *Energy Technology*, **2019**, 7, 1801030	3.5	10
92	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	4	9
91	Machine Learning Optimization of the Collocation Point Set for Solving the Kohn-Sham Equation. *Journal of Physical Chemistry A*, **2019**, 123, 10631-10642	2.8	9
90	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	3.6	9
89	Computational design of small organic dyes with strong visible absorption by controlled quinoidization of the thiophene unit. *Chemical Physics Letters*, **2014**, 593, 14-19	2.5	9
88	Towards Accurate Spectroscopic Identification of Species at Catalytic Surfaces: Anharmonic Vibrations of Formate on AuPt. *Materials Research Society Symposia Proceedings*, **2012**, 1484, 1		9
87	Photofragment image analysis via pattern recognition. *Review of Scientific Instruments*, **2004**, 75, 2435-2445	1.7	9
86	Fluorination of pyrene-based organic semiconductors enhances the performance of light emitting diodes and halide perovskite solar cells. *Organic Electronics*, **2020**, 77, 105524	3.5	9
85	Using rectangular collocation with finite difference derivatives to solve electronic Schrödinger equation. *Journal of Chemical Physics*, **2018**, 149, 204105	3.9	9
84	Influence of the aggregate state on band structure and optical properties of C60 computed with different methods. *Journal of Chemical Physics*, **2018**, 148, 204301	3.9	9
83	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	0.7	8
82	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	3.6	8
81	Intramolecular mode coupling of the isotopomers of water: a non-scalar charge density-derived perspective. *Physical Chemistry Chemical Physics*, **2020**, 22, 2509-2520	3.6	8
80	Highly accurate local pseudopotentials of Li, Na, and Mg for orbital free density functional theory. *Chemical Physics Letters*, **2015**, 622, 99-103	2.5	8
79	Nonspectral Methods for Solving the Schrödinger Equation for Electronic and Vibrational Problems. *Journal of Physical Chemistry Letters*, **2011**, 2, 2193-2199	6.4	8

78	Theoretical analysis of the solvatochromism of organic dyes differing by the conjugation sequence. *Journal of Photonics for Energy*, **2012**, 2, 028001	1.2	8
77	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	7.9	8
76	Effect of organic cation states on electronic properties of mixed organic-inorganic halide perovskite clusters. *Physical Chemistry Chemical Physics*, **2019**, 21, 8161-8169	3.6	7
75	Insertion of Mono- vs. Bi- vs. Trivalent Atoms in Prospective Active Electrode Materials for Electrochemical Batteries: An ab Initio Perspective. *Energies*, **2017**, 10, 2061	3.1	7
74	A Comparative Computational Study of Li, Na, and Mg Insertion in □Sn. *Materials Research Society Symposia Proceedings*, **2014**, 1678, 1		7
73	Computational design of new organics dyes with improved solar absorbance for dye-sensitized solar cells. *MRS Communications*, **2013**, 3, 37-39	2.7	7
72	Roadmap on Machine Learning in Electronic Structure. *Electronic Structure*,	2.6	7
71	Investigation of thiophene flanked diketopyrrolopyrrole monomers with straight and branched alkyl chains and their electropolymerization study. *Journal of Materials Research*, **2017**, 32, 2707-2718	2.5	6
70	Indenofluorene-based-copolymers: Influence of electron-deficient benzothiadiazole (BT) and benzooxadiazole (BO) moieties on light emitting devices. *Organic Electronics*, **2019**, 70, 14-24	3.5	6
69	Effect of Nuclear Motion on Charge Transport in Fullerenes: A Combined Density Functional Tight Binding□Density Functional Theory Investigation. *Frontiers in Energy Research*, **2019**, 7,	3.8	6
68	A computational study of adsorption and vibrations of UF6 on graphene derivatives: Conditions for 2D enrichment. *Carbon*, **2015**, 81, 800-806	10.4	6
67	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	3.9	6
66	Lithium Attachment to C60 and Nitrogen- and Boron-Doped C60: A Mechanistic Study. *Materials*, **2019**, 12,	3.5	6
65	Addition to "On the Charge State of Titanium in Titanium Dioxide". *Journal of Physical Chemistry Letters*, **2017**, 8, 3945-3946	6.4	6
64	Shear-induced conformation change in □crystalline nylon6. *Applied Physics Letters*, **2014**, 105, 221910	3.4	6
63	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	3.4	6
62	CONUNDrum: A program for orbital-free density functional theory calculations. *Computer Physics Communications*, **2020**, 256, 107365	4.2	6
61	Sodium Interaction with Disodium Terephthalate Molecule: an Ab Initio Study. *MRS Advances*, **2016**, 1, 3579-3584	0.7	6

60	Ab initio modeling and design of vanadia-based electrode materials for post-lithium batteries. *Journal Physics D: Applied Physics*, **2020**, 53, 083001	3	6
59	Defects in crystalline PVDF: a density functional theory-density functional tight binding study. *Physical Chemistry Chemical Physics*, **2017**, 19, 7560-7567	3.6	5
58	A Scheme for Ultrasensitive Detection of Molecules with Vibrational Spectroscopy in Combination with Signal Processing. *Molecules*, **2019**, 24,	4.8	5
57	First-Principle Insights Into Molecular Design for High-Voltage Organic Electrode Materials for Mg Based Batteries. *Frontiers in Chemistry*, **2020**, 8, 83	5	5
56	Reply to the Comment on "Revisiting backbonding: the influence of d orbitals on metal-CO bonds and ligand red shifts" by G. Frenking and S. Pan, Phys. Chem. Chem. Phys., 2019, 22, DOI. *Physical Chemistry Chemical Physics*, **2020**, 22, 5380-5382	3.6	5
55	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	3.5	5
54	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	3.5	5
53	A comparative computational study of the diffusion of Na and Li atoms in Sn(111) nanosheets. *Solid State Ionics*, **2014**, 268, 273-276	3.3	5
52	Effects of Nuclear Vibrations on the Energetics of Polythiophene: Quantized Energy Molecular Dynamics. *Australian Journal of Chemistry*, **2013**, 66, 1021	1.2	5
51	Significant Improvement of Optoelectronic and Photovoltaic Properties by Incorporating Thiophene in a Solution-Processable D-A-D Modular Chromophore. *Molecules*, **2015**, 20, 21787-801	4.8	5
50	Li Storage on TCNE and TCNE-(Doped)-Graphene Complexes: a Computational Study. *Materials Research Society Symposia Proceedings*, **2014**, 1679, 1		5
49	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**,		5
48	Effect of nuclear vibrations, temperature, and orientation on injection and recombination conditions in amino-phenyl acid dyes on TiO 2 **2012**,		5
47	Materials Design and Optimization for Next-Generation Solar Cell and Light-Emitting Technologies. *Journal of Physical Chemistry Letters*, **2021**, 12, 4638-4657	6.4	5
46	A Comparative First-Principles Study of Lithium, Sodium and Magnesium Insertion Energetics in Brookite Titanium Dioxide. *MRS Advances*, **2019**, 4, 837-842	0.7	5
45	Inverse Multiquadratic Functions as the Basis for the Rectangular Collocation Method to Solve the Vibrational Schrdinger Equation. *Mathematics*, **2018**, 6, 253	2.3	5
44	The role of solvent charge donation in the stabilization of metal ions in aqueous solution. *MRS Communications*, **2018**, 8, 1139-1144	2.7	5
43	Computational design of small phenothiazine dyes for dye-sensitized solar cells by functionalizations affecting the thiophene unit. *Journal of Molecular Modeling*, **2015**, 21, 67	2	4

42	The role of weak interactions in characterizing peptide folding preferences using a QTAIM interpretation of the Ramachandran plot (?-?). *International Journal of Quantum Chemistry*, **2018**, 118, e25456	2.1	4
41	Defects in alpha and gamma crystalline nylon6: A computational study. *AIP Advances*, **2015**, 5, 107123	1.5	4
40	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	2.2	4
39	Theoretical analysis of the absorption spectra of organic dyes differing by the conjugation sequence: illusion of negative solvatochromism **2012**,		4
38	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	1.4	4
37	Effect of Isotopic Substitution on Elementary Processes in Dye-Sensitized Solar Cells: Deuterated Amino-Phenyl Acid Dyes on TiO2. *Computation*, **2013**, 1, 1-15	2.2	4
36	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	1.4	4
35	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	6.2	4
34	Nonparametric Local Pseudopotentials with Machine Learning: A Tin Pseudopotential Built Using Gaussian Process Regression. *Journal of Physical Chemistry A*, **2020**, 124, 11111-11124	2.8	4
33	One-step direct oxidation of fullerene-fused alkoxy ethers to ketones for evaporable fullerene derivatives. *Communications Chemistry*, **2021**, 4,	6.3	4
32	Grown-in beryllium diffusion in indium gallium arsenide: An ab initio, continuum theory and kinetic Monte Carlo study. *Acta Materialia*, **2017**, 125, 455-464	8.4	3
31	First-Principles Study of the Calcium Insertion in Layered and Non-Layered Phases of Vanadia. *MRS Advances*, **2018**, 3, 3507-3512	0.7	3
30	Achieving Improved Solar Absorbance of Small Organic Dyes Featuring Quinoidized Five-Membered Heterocycles. *Materials Research Society Symposia Proceedings*, **2014**, 1667, 26		3
29	Computational study of Mg insertion into amorphous silicon: advantageous energetics over crystalline silicon for Mg storage. *Materials Research Society Symposia Proceedings*, **2013**, 1540, 3601		3
28	Configuration of ring-down spectrometers for maximum sensitivity. *Canadian Journal of Chemistry*, **2004**, 82, 873-879	0.9	3
27	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	5.1	3
26	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	4.2	3
25	Versatile nature of anthanthrone based polymers as active multifunctional semiconductors for various organic electronic devices. *Materials Advances*, **2020**, 1, 3428-3438	3.3	3

24	A Model for Estimating Chemical Potentials in Ternary Semiconductor Compounds: the Case of InGaAs. *MRS Advances*, **2017**, 2, 2909-2914	0.7	2
23	Aggregate-State Effects in the Atomistic Modeling of Organic Materials for Electrochemical Energy Conversion and Storage Devices: A Perspective. *Molecules*, **2020**, 25,	4.8	2
22	Dopant-dopant interactions in beryllium doped indium gallium arsenide: An ab initio study. *Journal of Materials Research*, **2018**, 33, 401-413	2.5	2
21	Effect of the adsorption of ethylene carbonate on Si surfaces on the Li insertion behavior. *Chemical Physics Letters*, **2013**, 585, 157-161	2.5	2
20	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		2
19	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	0.3	2
18	Pyrrolo[3,2-]pyrrole-1,4-dione (IsoDPP) End Capped with Napthalimide or Phthalimide: Novel Small Molecular Acceptors for Organic Solar Cells. *Molecules*, **2020**, 25,	4.8	2
17	Modeling of plasmonic properties of nanostructures for next generation solar cells and beyond. *Advances in Physics: X*, **2021**, 6, 1908848	5.1	2
16	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	2.7	1
15	Electrochemical Performance of B-Type Vanadium Dioxide as a Sodium-Ion Battery Cathode: A Combined Experimental and Theoretical Study. *ChemElectroChem*, **2020**, 7, 3151-3159	4.3	1
14	Reflections of a Computer Poet on American Social Dynamics (Or How This Makes Sense). *Advances in Literary Study*, **2014**, 02, 47-57	0	1
13	Oxygen Redox Activity in Cathodes: A Common Phenomenon Calling for Density-Based Descriptors. *Journal of Physical Chemistry C*, **2020**, 124, 19962-19968	3.8	1
12	Effect of Surface Treatment on the Mode I Debonding of Interface Between Silica and Nylon6. *MRS Advances*, **2016**, 1, 2717-2722	0.7	1
11	Mg and K Insertion in Glassy Amorphous Carbon vs Graphite as Potential Anode Materials: an Ab Initio Study. *MRS Advances*, **2016**, 1, 3069-3074	0.7	1
10	Structural Geometry Variation of 1,4-Naphthalene-Based Co-Polymers to Tune the Device Performance of PVK-Host-Based OLEDs. *Polymers*, **2021**, 13,	4.5	1
9	Carbon/air secondary battery system and demonstration of its charge-discharge. *Journal of Power Sources*, **2021**, 516, 230681	8.9	0
8	Naphthalene Flanked Diketopyrrolopyrrole: A New Functional Dye Based Optical Sensors for Monitoring Cyanide Ions in Water. *Advanced Materials Technologies*,2100170	6.8	0
7	Can doping of transition metal oxide cathode materials increase achievable voltages with multivalent metals?. *International Journal of Quantum Chemistry*, **2021**, 121, e26439	2.1	0

List of Publications

6	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	First-Principles Study of the Electrochemical Sodiation of Rutile-Type Vanadium Dioxide. *MRS Advances*, **2020**, 5, 1467-1474	0.7
4	Adsorption of UF 6 on Graphene Derivatives: a Computational Study of Conditions for 2D Enrichment. *Materials Research Society Symposia Proceedings*, **2014**, 1683, 32	
3	Modeling Methods for Plasmonic Effects in Halide Perovskite Based Systems for Photonics Applications **2021**, 1-52	
2	Adsorption and Light Absorption Properties of 2-Anthroic Acid on Titania: a Density Functional Theory Time-Dependent Density Functional Theory Study. *MRS Advances*, **2016**, 1, 2795-2800	0.7
1	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	6.8