Francoise Remacle

List of Publications by Year in Descending Order

269 papers	6,764 citations	42 h-index	70 g-index
291 ext. papers	7,401 ext. citations	4.9 avg, IF	6.05 L-index

#	Paper	IF	Citations
269	Compacting the density matrix in quantum dynamics: Singular value decomposition of the surprisal and the dominant constraints for anharmonic systems. *Journal of Chemical Physics*, **2021**, 155, 204110	3.9	0
268	Ellipticity controlled dissociative double ionization of ethane by strong fields. *Physical Chemistry Chemical Physics*, **2021**, 23, 23537-23543	3.6	2
267	Electronic Coherences Steer the Strong Isotope Effect in the Ultrafast Jahn-Teller Structural Rearrangement of Methane Cation upon Tunnel Ionization. *Journal of Physical Chemistry A*, **2021**, 125, 9495-9507	2.8	1
266	Identification of an ultrafast internal conversion pathway of pyrazine by time-resolved vacuum ultraviolet photoelectron spectrum simulations. *Journal of Chemical Physics*, **2021**, 154, 224304	3.9	2
265	The density matrix via few dominant observables: The quantum interference in the isotope effect for atto-pumped N. *Journal of Chemical Physics*, **2021**, 155, 024109	3.9	2
264	DNA-based constitutional dynamic networks as functional modules for logic gates and computing circuit operations. *Chemical Science*, **2021**, 12, 5473-5483	9.4	4
263	Ultrafast fs coherent excitonic dynamics in CdSe quantum dots assemblies addressed and probed by 2D electronic spectroscopy. *Journal of Chemical Physics*, **2021**, 154, 014301	3.9	4
262	Ultrafast geometrical reorganization of a methane cation upon sudden ionization: an isotope effect on electronic non-equilibrium quantum dynamics. *Physical Chemistry Chemical Physics*, **2021**, 23, 12051-12059	3.6	7
261	Chirality of a rhodamine heterodimer linked to a DNA scaffold: an experimental and computational study. *Physical Chemistry Chemical Physics*, **2020**, 22, 7516-7523	3.6	0
260	Correlated electron–nuclear motion during non-adiabatic transitions in LiH and its isotopomers. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2020**, 53, 134001	1.3	5
259	Room-Temperature Inter-Dot Coherent Dynamics in Multilayer Quantum Dot Materials. *Journal of Physical Chemistry C*, **2020**, 124, 16222-16231	3.8	13
258	Coherent Exciton Dynamics in Ensembles of Size-Dispersed CdSe Quantum Dot Dimers Probed via Ultrafast Spectroscopy: A Quantum Computational Study. *Applied Sciences (Switzerland)*, **2020**, 10, 1328	2.6	8
257	Parallel Quantum Computation of Vibrational Dynamics. *Frontiers in Physics*, **2020**, 8,	3.9	2
256	Surprisal of a quantum state: Dynamics, compact representation, and coherence effects. *Journal of Chemical Physics*, **2020**, 153, 214105	3.9	3
255	Selective bond formation triggered by short optical pulses: quantum dynamics of a four-center ring closure. *Physical Chemistry Chemical Physics*, **2020**, 22, 22302-22313	3.6	7
254	Thermodynamic energetics underlying genomic instability and whole-genome doubling in cancer. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 18880-18890	11.5	2
253	Quantum Device Emulates the Dynamics of Two Coupled Oscillators. *Journal of Physical Chemistry Letters*, **2020**, 11, 6990-6995	6.4	9

252	Massively parallel classical logic via coherent dynamics of an ensemble of quantum systems with dispersion in size. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 21022-21030	11.5	7
251	Intracellular redox potential is correlated with miRNA expression in MCF7 cells under hypoxic conditions. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 19753-19759	11.5	9
250	Sub-Femtosecond Stark Control of Molecular Photoexcitation with Near Single-Cycle Pulses. *Journal of Physical Chemistry Letters*, **2019**, 10, 742-747	6.4	7
249	Consecutive feedback-driven constitutional dynamic networks. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 2843-2848	11.5	25
248	Understanding chemical interaction between phosphonate-derivative molecules and a silver surface cluster in SERS: a combined experimental and computational approach. *Physical Chemistry Chemical Physics*, **2019**, 21, 22180-22187	3.6	5
247	Temporal and spatially resolved imaging of the correlated nuclear-electronic dynamics and of the ionized photoelectron in a coherently electronically highly excited vibrating LiH molecule. *Journal of Chemical Physics*, **2019**, 151, 134310	3.9	8
246	Time resolved mechanism of the isotope selectivity in the ultrafast light induced dissociation in N. *Journal of Chemical Physics*, **2019**, 151, 114308	3.9	3
245	Metabolic, Physiological, and Transcriptomics Analysis of Batch Cultures of the Green Microalga Grown on Different Acetate Concentrations. *Cells*, **2019**, 8,	7.9	11
244	Quantum Phenomena in Nanomaterials: Coherent Superpositions of Fine Structure States in CdSe Nanocrystals at Room Temperature. *Journal of Physical Chemistry C*, **2019**, 123, 31286-31293	3.8	20
243	Angle-resolved photoelectron spectroscopy and scanning tunnelling spectroscopy studies of the endohedral fullerene Li@C. *Nanoscale*, **2019**, 11, 2668-2678	7.7	12
242	Fast Energy Transfer in CdSe Quantum Dot Layered Structures: Controlling Coupling with Covalent-Bond Organic Linkers. *Journal of Physical Chemistry C*, **2018**, 122, 5753-5758	3.8	18
241	Propagation of nonstationary electronic and nuclear states: attosecond dynamics in LiF. *Molecular Physics*, **2018**, 116, 2524-2532	1.7	2
240	On the fly quantum dynamics of electronic and nuclear wave packets. *Chemical Physics Letters*, **2018**, 699, 155-161	2.5	4
239	Gas-Phase Photoluminescence and Photodissociation of Silver-Capped Hexagold Clusters. *Journal of Physical Chemistry A*, **2018**, 122, 5799-5810	2.8	7
238	Ultrafast nonradiative transition pathways in photo-excited pyrazine: Ab initio analysis of time-resolved vacuum ultraviolet photoelectron spectrum. *Chemical Physics*, **2018**, 515, 704-709	2.3	8
237	Multivalued Logic at the Nanoscale. *Natural Computing Series*, **2018**, 295-318	2.5	2
236	Computing by Non-linear Optical Molecular Response. *Natural Computing Series*, **2018**, 45-53	2.5	
235	Surprisal analysis of the transcriptomic response of the green microalga Chlamydomonas to the addition of acetate during day/night cycles. *Chemical Physics*, **2018**, 514, 154-163	2.3	2

234	Surprisal analysis of genome-wide transcript profiling identifies differentially expressed genes and pathways associated with four growth conditions in the microalga Chlamydomonas. *PLoS ONE*, **2018**, 13, e0195142	3.7	6
233	RNA-seq data and surprisal analysis of mutant and control strain of the green microalga during day/night cycles. *Data in Brief*, **2018**, 21, 351-353	1.2	
232	This special thematic issue of chemical physics Energy and entropy of change: From elementary processes to biology celebrates the 80th birthday of Prof. Raphael D. Levine, known as Raphy. *Chemical Physics*, **2018**, 514, 1-3	2.3	
231	Time-dependent view of an isotope effect in electron-nuclear nonequilibrium dynamics with applications to N. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 5890-5895	11.5	11
230	Personalized disease signatures through information-theoretic compaction of big cancer data. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 7694-7699	11.5	14
229	Intercommunication of DNA-Based Constitutional Dynamic Networks. *Journal of the American Chemical Society*, **2018**, 140, 8721-8731	16.4	32
228	Nuclear Motion Driven Ultrafast Photodissociative Charge Transfer of the PENNA Cation: An Experimental and Computational Study. *Journal of Physical Chemistry A*, **2017**, 121, 1442-1447	2.8	10
227	A Probabilistic Finite State Logic Machine Realized Experimentally on a Single Dopant Atom. *Nano Letters*, **2017**, 17, 1846-1852	11.5	7
226	Implementation of Multivariable Logic Functions in Parallel by Electrically Addressing a Molecule of Three Dopants in Silicon. *ChemPhysChem*, **2017**, 18, 1790-1797	3.2	3
225	Implementation of Probabilistic Algorithms by Multi-chromophoric Molecular Networks with Application to Multiple Travelling Pathways. *ChemPhysChem*, **2017**, 18, 1782-1789	3.2	2
224	A new electron-ion coincidence 3D momentum-imaging method and its application in probing strong field dynamics of 2-phenylethyl-N, N-dimethylamine. *Journal of Chemical Physics*, **2017**, 147, 013920	3.9	10
223	Continuous variables logic coupled automata using a DNAzyme cascade with feedback. *Chemical Science*, **2017**, 8, 2161-2168	9.4	21
222	Spatial and temporal control of populations, branching ratios, and electronic coherences in LiH by a single one-cycle infrared pulse. *Physical Review A*, **2017**, 95,	2.6	16
221	Optical activity of the super-atom molecular orbital (SAMO) states in Li@C60+ conformers **2017**,		1
220	The Role of Super-Atom Molecular Orbitals in Doped Fullerenes in a Femtosecond Intense Laser Field. *Journal of Physics: Conference Series*, **2017**, 875, 032017	0.3	
219	Low-lying, Rydberg states of polycyclic aromatic hydrocarbons (PAHs) and cyclic alkanes. *Physical Chemistry Chemical Physics*, **2017**, 19, 24090-24099	3.6	11
218	Where Ion Mobility and Molecular Dynamics Meet To Unravel the (Un)Folding Mechanisms of an Oligorotaxane Molecular Switch. *ACS Nano*, **2017**, 11, 10253-10263	16.7	18
217	The Role of Super-Atom Molecular Orbitals in Doped Fullerenes in a Femtosecond Intense Laser Field. *Scientific Reports*, **2017**, 7, 121	4.9	6

216	Coherent electronic and nuclear dynamics in a rhodamine heterodimer-DNA supramolecular complex. *Physical Chemistry Chemical Physics*, **2017**, 19, 23043-23051	3.6	20
215	Photoinduced Ultrafast Charge Transfer and Charge Migration in Small Gold Clusters Passivated by a Chromophoric Ligand. *Nano Letters*, **2017**, 17, 5672-5681	11.5	5
214	Ultrafast 25-fs relaxation in highly excited states of methyl azide mediated by strong nonadiabatic coupling. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E11072-E11081	11.5	12
213	Pumping and probing vibrational modulated coupled electronic coherence in HCN using short UV fs laser pulses: a 2D quantum nuclear dynamical study. *Physical Chemistry Chemical Physics*, **2017**, 19, 19837-19846	2.6	3
212	Electronic states and valley-orbit coupling in linear and planar molecules formed by coupled P donors in silicon. *Physical Review B*, **2017**, 95,	3.3	6
211	Electronic and Nuclear Dynamics for a Non-Equilibrium Electronic State: The Ultrafast Pumping of N2. *Progress in Theoretical Chemistry and Physics*, **2017**, 195-208	0.6	2
210	Controlling Coherent Quantum Nuclear Dynamics in LiH by Ultra Short IR Atto Pulses. *Springer Series in Chemical Physics*, **2017**, 41-65	0.3	1
209	Multivariate Surprisal Analysis of Gene Expression Levels. *Entropy*, **2016**, 18, 445	2.8	3
208	Experimental and Theoretical Study of the Reactivity of Gold Nanoparticles Towards Benzimidazole-2-ylidene Ligands. *Chemistry - A European Journal*, **2016**, 22, 10446-58	4.8	27
207	Transition from SAMO to Rydberg State Ionization in C in Femtosecond Laser Fields. *Journal of Physical Chemistry Letters*, **2016**, 7, 4677-4682	6.4	13
206	Quantum Nuclear Dynamics Pumped and Probed by Ultrafast Polarization Controlled Steering of a Coherent Electronic State in LiH. *Journal of Physical Chemistry A*, **2016**, 120, 3343-52	2.8	20
205	Probing in Space and Time the Nuclear Motion Driven by Nonequilibrium Electronic Dynamics in Ultrafast Pumped N2. *Journal of Physical Chemistry A*, **2016**, 120, 3335-42	2.8	11
204	Time-efficient computation of the electronic structure of the C60 super-atom molecular orbital (SAMO) states in TDDFT **2016**,		3
203	Operation of a quantum dot in the finite-state machine mode: Single-electron dynamic memory. *Journal of Applied Physics*, **2016**, 120, 024503	2.5	2
202	Force measurements reveal how small binders perturb the dissociation mechanisms of DNA duplex sequences. *Nanoscale*, **2016**, 8, 11718-26	7.7	8
201	Coherent electronic wave packet motion in C(60) controlled by the waveform and polarization of few-cycle laser fields. *Physical Review Letters*, **2015**, 114, 123004	7.4	46
200	Computational Benchmarking for Ultrafast Electron Dynamics: Wave Function Methods vs Density Functional Theory. *Journal of Chemical Theory and Computation*, **2015**, 11, 2221-33	6.4	10
199	Parallel and Multivalued Logic by the Two-Dimensional Photon-Echo Response of a RhodamineDNA Complex. *Journal of Physical Chemistry Letters*, **2015**, 6, 1714-8	6.4	20

198	Ternary DNA computing using 3 □3 multiplication matrices. *Chemical Science*, **2015**, 6, 1288-1292	9.4	36
197	Metabolomic analysis of the green microalga Chlamydomonas reinhardtii cultivated under day/night conditions. *Journal of Biotechnology*, **2015**, 215, 20-6	3.7	23
196	Statistical thermodynamics of transcription profiles in normal development and tumorigeneses in cohorts of patients. *European Biophysics Journal*, **2015**, 44, 709-26	1.9	8
195	Measurement and laser control of attosecond charge migration in ionized iodoacetylene. *Science*, **2015**, 350, 790-5	33.3	352
194	Multivalley envelope function equations and effective potentials for phosphorus impurity in silicon. *Physical Review B*, **2015**, 92,	3.3	8
193	Information processing in parallel through directionally resolved molecular polarization components in coherent multidimensional spectroscopy. *Journal of Chemical Physics*, **2015**, 143, 064106	3.9	8
192	Ultrafast dynamics in the bifunctional PENNA neutral and cation molecule induced by ultrashort photoexcitation. *Journal of Physics: Conference Series*, **2015**, 635, 112068	0.3	
191	Photoinduced Ultrafast Electronic Dynamics in Polyatomic Molecules: A time-dependent computational study. *Journal of Physics: Conference Series*, **2015**, 635, 112066	0.3	1
190	Attosecond charge migration and its laser control. *Journal of Physics: Conference Series*, **2015**, 635, 112136	0.3	1
189	An Atomistic View of DNA Dynamics and Its Interaction with Small Binders: Insights from Molecular Dynamics and Principal Component Analysis. *Advances in Atom and Single Molecule Machines*, **2015**, 17-33	0	1
188	Relative Photoionization Cross Sections of Super-Atom Molecular Orbitals (SAMOs) in C60. *Journal of Physical Chemistry A*, **2015**, 119, 11504-8	2.8	11
187	Charge Redistribution Effects on the UV□Vis Spectra of Small Ligated Gold Clusters: a Computational Study. *Journal of Physical Chemistry C*, **2015**, 119, 10969-10980	3.8	30
186	Electronic states and wavefunctions of diatomic donor molecular ions in silicon: multi-valley envelope function theory. *Journal of Physics Condensed Matter*, **2014**, 26, 065302	1.8	8
185	AttoPhotoChemistry. Probing ultrafast electron dynamics by the induced nuclear motion: The prompt and delayed predissociation of N2. *Chemical Physics Letters*, **2014**, 601, 45-48	2.5	9
184	Glioblastoma cellular architectures are predicted through the characterization of two-cell interactions. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 6521-6	11.5	44
183	A full-adder based on reconfigurable DNA-hairpin inputs and DNAzyme computing modules. *Chemical Science*, **2014**, 5, 3381	9.4	69
182	DNAzyme-based 2:1 and 4:1 multiplexers and 1:2 demultiplexer. *Chemical Science*, **2014**, 5, 1074	9.4	74
181	Electronic dynamics by ultrafast pump photoelectron detachment probed by ionization: a dynamical simulation of negative-neutral-positive in LiH(-). *Journal of Physical Chemistry A*, **2014**, 118, 6721-9	2.8	14

180	Atomistic account of structural and dynamical changes induced by small binders in the double helix of a short DNA. *Physical Chemistry Chemical Physics*, **2014**, 16, 14070-82	3.6	17
179	Charge migration in the bifunctional PENNA cation induced and probed by ultrafast ionization: a dynamical study. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2014**, 47, 124011	1.3	51
178	Tuning the Properties of Pd Nanoclusters by Ligand Coatings: Electronic Structure Computations on Phosphine, Thiol, and Mixed Phosphine–Thiol Ligand Shells. *Journal of Physical Chemistry C*, **2014**, 118, 9790-9800	3.8	16
177	Ligand and Solvation Effects on the Structural and Electronic Properties of Small Gold Clusters. *Journal of Physical Chemistry C*, **2014**, 118, 4362-4376	3.8	33
176	Surprisal analysis of Glioblastoma Multiform (GBM) microRNA dynamics unveils tumor specific phenotype. *PLoS ONE*, **2014**, 9, e108171	3.7	7
175	Computational surprisal analysis speeds-up genomic characterization of cancer processes. *PLoS ONE*, **2014**, 9, e108549	3.7	3
174	Control of electronic dynamics visualized by angularly resolved photoelectron spectra: A dynamical simulation with an IR pump and XUV attosecond-pulse-train probe. *Physical Review A*, **2014**, 89,	2.6	26
173	Quantum dot ternary-valued full-adder: Logic synthesis by a multiobjective design optimization based on a genetic algorithm. *Journal of Applied Physics*, **2014**, 116, 164316	2.5	4
172	Pump and probe of ultrafast charge reorganization in small peptides: a computational study through sudden ionizations. *Journal of Physical Chemistry A*, **2013**, 117, 10513-25	2.8	28
171	Molecular decision trees realized by ultrafast electronic spectroscopy. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 17183-8	11.5	21
170	miRNA and mRNA cancer signatures determined by analysis of expression levels in large cohorts of patients. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 19160-5	11.5	57
169	Hot electron production and diffuse excited states in C70, C82, and Sc3N@C80 characterized by angular-resolved photoelectron spectroscopy. *Journal of Chemical Physics*, **2013**, 139, 084309	3.9	15
168	Free energy rhythms in Saccharomyces cerevisiae: a dynamic perspective with implications for ribosomal biogenesis. *Biochemistry*, **2013**, 52, 1641-8	3.2	9
167	Hypoxia induces a phase transition within a kinase signaling network in cancer cells. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, E1352-60	11.5	55
166	Probing rapidly-ionizing super-atom molecular orbitals in C60: a computational and femtosecond photoelectron spectroscopy study. *ChemPhysChem*, **2013**, 14, 3332-40	3.2	25
165	Realization of Complex Logic Operations at the Nanoscale. *Advances in Atom and Single Molecule Machines*, **2013**, 195-220	0	3
164	Imaging Orbitals by Ionization or Electron Attachment: The Role of Dyson Orbitals. *Advances in Atom and Single Molecule Machines*, **2013**, 41-54	0	11
163	pH-programmable DNA logic arrays powered by modular DNAzyme libraries. *Nano Letters*, **2012**, 12, 6049-54	11.5	96

162	Ultrafast predissociation mechanism of the 1Πu states of 14N2 and its isotopomers upon attosecond excitation from the ground state. *Journal of Physical Chemistry A*, **2012**, 116, 11311-8	2.8	16
161	Localized electron dynamics in attosecond-pulse-excited molecular systems: Probing the time-dependent electron density by sudden photoionization. *Physical Review A*, **2012**, 86,	2.6	49
160	Logic reversibility and thermodynamic irreversibility demonstrated by DNAzyme-based Toffoli and Fredkin logic gates. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 21228-33	11.5	77
159	Stabilization of merocyanine by protonation, charge, and external electric fields and effects on the isomerization of spiropyran: a computational study. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	10
158	Magnetostructural effects in ligand stabilized Pd13 clusters: a density functional theory study. *Nanoscale*, **2012**, 4, 4138-47	7.7	17
157	On a fundamental structure of gene networks in living cells. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 4702-7	11.5	42
156	Interplay of structural and electronic stabilizing factors in neutral and cationic phosphine protected Au13 clusters. *European Physical Journal D*, **2012**, 66, 1	1.3	16
155	Querying a quasi-classical Oracle: One-bit function identification problem implemented in a single atom transistor. *Europhysics Letters*, **2012**, 99, 28004	1.6	2
154	Angular-resolved photoelectron spectroscopy of superatom orbitals of fullerenes. *Physical Review Letters*, **2012**, 108, 173401	7.4	36
153	Maximal entropy multivariate analysis. *Molecular Physics*, **2012**, 110, 1659-1668	1.7	
152	20-Nanogold Au20(Td) and Low-Energy Hollow Cages: Void Reactivity. *Progress in Theoretical Chemistry and Physics*, **2012**, 571-598	0.6	
151	Protein signaling networks from single cell fluctuations and information theory profiling. *Biophysical Journal*, **2011**, 100, 2378-86	2.9	50
150	Balanced ternary addition using a gated silicon nanowire. *Applied Physics Letters*, **2011**, 99, 263109	3.4	7
149	Logic operations in a doped solid driven by stimulated Raman adiabatic passage. *Physical Review A*, **2011**, 83,	2.6	13
148	Whose Entropy: A Maximal Entropy Analysis of Phosphorylation Signaling. *Journal of Statistical Physics*, **2011**, 144, 429-442	1.5	2
147	Convergence of logic of cellular regulation in different premalignant cells by an information theoretic approach. *BMC Systems Biology*, **2011**, 5, 42	3.5	24
146	Stereocontrol of attosecond time-scale electron dynamics in ABCU using ultrafast laser pulses: a computational study. *Physical Chemistry Chemical Physics*, **2011**, 13, 8331-44	3.6	31
145	Integrated logic circuits using single-atom transistors. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 13969-72	11.5	31

144	Attosecond pumping of nonstationary electronic states of LiH: Charge shake-up and electron density distortion. *Physical Review A*, **2011**, 83,	2.6	38
143	On the strong and selective isotope effect in the UV excitation of N2 with implications toward the nebula and Martian atmosphere. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 6020-5	11.5	43
142	Logic implementations using a single nanoparticle-protein hybrid. *Nature Nanotechnology*, **2010**, 5, 451-7	28.7	29
141	DNA computing circuits using libraries of DNAzyme subunits. *Nature Nanotechnology*, **2010**, 5, 417-22	28.7	369
140	All-DNA finite-state automata with finite memory. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 21996-2001	11.5	112
139	Ternary logic implemented on a single dopant atom field effect silicon transistor. *Applied Physics Letters*, **2010**, 96, 043107	3.4	22
138	Maximal entropy inference of oncogenicity from phosphorylation signaling. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 6112-7	11.5	9
137	DFT Studies of Solvation Effects on the Nanosize Bare, Thiolated, and Redox Active Ligated Au55 Cluster *Journal of Physical Chemistry C*, **2010**, 114, 15941-15950	3.8	10
136	Information-theoretic analysis of phenotype changes in early stages of carcinogenesis. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 10324-9	11.5	59
135	Electrically Addressing a Molecule-Like Donor Pair in Silicon: An Atomic Scale Cyclable Full Adder Logic. *Journal of Physical Chemistry C*, **2010**, 114, 20380-20386	3.8	8
134	Controlled full adder-subtractor by vibrational computing. *Physical Chemistry Chemical Physics*, **2010**, 12, 15628-35	3.6	9
133	20-nanogold Au20(Td) cluster and its hollow cage isomers: structural and energetic properties. *Journal of Physics: Conference Series*, **2010**, 248, 012026	0.3	2
132	Redox-Executed Logic Operations through the Reversible Voltammetric Response Characteristics of Electroactive Self-Assembled Monolayers. *Australian Journal of Chemistry*, **2010**, 63, 173	1.2	7
131	Gas phase fullerene anions hydrogenation by methanol followed by IRMPA dehydrogenation. *Journal of the American Society for Mass Spectrometry*, **2010**, 21, 117-26	3.5	3
130	Bonding patterns of [Ag2-alanine]0, hybrid complexes and the implementation of molecular logic gates. *International Journal of Quantum Chemistry*, **2010**, 110, 2237-2246	2.1	28
129	Controlled full adder or subtractor by vibrational quantum computing. *Physical Review A*, **2009**, 80,	2.6	12
128	The post-Born Oppenheimer regime: dynamics of electronic motion in molecules by attosecond few-cycle spectroscopy. *Physica Scripta*, **2009**, 80, 048101	2.6	25
127	Electrochemically driven sequential machines: an implementation of copper rotaxanes. *Chemistry - A European Journal*, **2009**, 15, 1310-3	4.8	95

126	Reconfigurable logic devices on a single dopant atom - operation up to a full adder by using electrical spectroscopy. *ChemPhysChem*, **2009**, 10, 162-73	3.2	19
125	Electronic wave packet motion in water dimer cation: A many electron description. *Chemical Physics* , **2009**, 366, 129-138	2.3	47
124	Computational, structural, and mechanistic analysis of the electrochemically driven pirouetting motion of a copper rotaxane. *Journal of Physical Chemistry B*, **2009**, 113, 6219-29	3.4	19
123	Combined Mössbauer spectral and density functional theory determination of the magnetic easy-axis in two high-spin iron(II) 2-pyrazinecarboxylate complexes. *Inorganic Chemistry*, **2009**, 48, 8173-9	5.1	10
122	Ligand and solvation effects on the electronic properties of Au55 clusters: a density functional theory study. *Nano Letters*, **2009**, 9, 3007-11	11.5	35
121	The elimination of redundant constraints in surprisal analysis of unimolecular dissociation and other endothermic processes. *Journal of Physical Chemistry A*, **2009**, 113, 4658-64	2.8	5
120	Vibrational computing: simulation of a full adder by optimal control. *Journal of Chemical Physics*, **2008**, 128, 064110	3.9	31
119	Pump and probe ultrafast electron dynamics in LiH: a computational study. *New Journal of Physics*, **2008**, 10, 025019	2.9	83
118	All Optical Full Adder Based on Intramolecular Electronic Energy Transfer in the Rhodamine–Azulene Bichromophoric System. *Journal of Physical Chemistry C*, **2008**, 112, 15880-15885	3.8	19
117	A density functional theory calculation of the electronic properties of several high-spin and low-spin iron(II) pyrazolylborate complexes. *Inorganic Chemistry*, **2008**, 47, 4005-14	5.1	25
116	Principles of design of a set-reset finite state logic nanomachine. *Journal of Applied Physics*, **2008**, 104, 044509	2.5	12
115	Computational investigation and experimental considerations for the classical implementation of a full adder on SO2 by optical pump-probe schemes. *Journal of Chemical Physics*, **2008**, 128, 194308	3.9	4
114	Implementation of simple logic gates on gold–ammonia bonding patterns in different charge states. *Molecular Physics*, **2008**, 106, 521-530	1.7	8
113	Ultrafast vibrational spectroscopy and relaxation in polyatomic molecules: Potential for molecular parallel computing. *Chemical Physics*, **2008**, 347, 531-545	2.3	11
112	Transcending binary logic by gating three coupled quantum dots. *Nano Letters*, **2007**, 7, 2795-9	11.5	29
111	Time-Resolved Electrochemical Spectroscopy of Charge Migration in Molecular Wires: Computational Evidence for Rich Electronic Dynamics. *Journal of Physical Chemistry C*, **2007**, 111, 2301-2309	3.8	8
110	The Emergence of a Coupled Quantum Dot Array in a Doped Silicon Nanowire Gated by Ultrahigh Density Top Gate Electrodes *Journal of Physical Chemistry C*, **2007**, 111, 17852-17860	3.8	3
109	Charge Distribution in 3?-Deoxythymidine-Fullerene: Mass Spectrometry, Laser Excitation, and Computational Studies. *Israel Journal of Chemistry*, **2007**, 47, 25-35	3.4	0

108	On the feasibility of an ultrafast purely electronic reorganization in lithium hydride. *Chemical Physics*, **2007**, 338, 342-347	2.3	39
107	The magic gold cluster Au20. *International Journal of Quantum Chemistry*, **2007**, 107, 2922-2934	2.1	80
106	Towards parallel computing: representation of a linear finite state digital logic machine by a molecular relaxation process. *European Physical Journal D*, **2007**, 42, 49-59	1.3	5
105	Chapter 11 Small gold clusters form nonconventional hydrogen bonds X-H ? Au: gold-water clusters as example. *Theoretical and Computational Chemistry*, **2007**, 19, 219-250		2
104	The gold-ammonia bonding patterns of neutral and charged complexes Au m 0+/-1-(NH3)n. I. Bonding and charge alternation. *Journal of Chemical Physics*, **2007**, 127, 194305	3.9	40
103	Probing Ultrafast Purely Electronic Charge Migration in Small Peptides. *Zeitschrift Fur Physikalische Chemie*, **2007**, 221, 647-661	3.1	47
102	Laser steered ultrafast quantum dynamics of electrons in LiH. *Physical Review Letters*, **2007**, 99, 183902	7.4	110
101	The time scale for electronic reorganization upon sudden ionization of the water and water-methanol hydrogen bonded dimers and of the weakly bound NO dimer. *Journal of Chemical Physics*, **2006**, 125, 133321	3.9	24
100	All-optical digital logic: Full addition or subtraction on a three-state system. *Physical Review A*, **2006** , 73,	2.6	39
99	An electronic time scale in chemistry. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 6793-8	11.5	305
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