Wolfgang Wenzel

List of Publications by Citations

269 papers	7,104 citations	45 h-index	67 g-index
299 ext. papers	8,062 ext. citations	6.6 avg, IF	6.1 L-index

#	Paper	IF	Citations
269	Mutations in CHD7, encoding a chromatin-remodeling protein, cause idiopathic hypogonadotropic hypogonadism and Kallmann syndrome. *American Journal of Human Genetics*, **2008**, 83, 511-9	11	256
268	Electrical transport through single-molecule junctions: from molecular orbitals to conduction channels. *Physical Review Letters*, **2002**, 88, 256803	7.4	214
267	Simulating charge transport in tris(8-hydroxyquinoline) aluminium (Alq(3)). *Physical Chemistry Chemical Physics*, **2008**, 10, 1852-8	3.6	155
266	Charge-Transfer-Induced Lattice Collapse in Ni-Rich NCM Cathode Materials during Delithiation. *Journal of Physical Chemistry C*, **2017**, 121, 24381-24388	3.8	148
265	Stochastic Tunneling Approach for Global Minimization of Complex Potential Energy Landscapes. *Physical Review Letters*, **1999**, 82, 3003-3007	7.4	147
264	WDR11, a WD protein that interacts with transcription factor EMX1, is mutated in idiopathic hypogonadotropic hypogonadism and Kallmann syndrome. *American Journal of Human Genetics*, **2010**, 87, 465-79	11	134
263	Selective dispersion of single-walled carbon nanotubes with specific chiral indices by poly(N-decyl-2,7-carbazole). *Journal of the American Chemical Society*, **2011**, 133, 652-5	16.4	126
262	Characterization of unstable periodic orbits in chaotic attractors and repellers. *Physical Review Letters*, **1989**, 63, 819-822	7.4	101
261	Current collapse in tunneling transport through benzene. *Physical Review Letters*, **2003**, 90, 076805	7.4	100
260	Mott-Hubbard metal-insulator transition in nonbipartite lattices. *Physical Review Letters*, **1990**, 64, 950-953	7.4	95
259	Reproducible protein folding with the stochastic tunneling method. *Physical Review Letters*, **2003**, 91, 158102	7.4	93
258	Interfacial dominated ferromagnetism in nanograined ZnO: a ESR and DFT study. *Scientific Reports*, **2015**, 5, 8871	4.9	92
257	Ab Initio Treatment of Disorder Effects in Amorphous Organic Materials: Toward Parameter Free Materials Simulation. *Journal of Chemical Theory and Computation*, **2014**, 10, 3720-5	6.4	87
256	Wavelength-Gated Dynamic Covalent Chemistry. *Angewandte Chemie - International Edition*, **2018**, 57, 2036-2045	16.4	83
255	Switching the Proton Conduction in Nanoporous, Crystalline Materials by Light. *Advanced Materials*, **2018**, 30, 1706551	24	78
254	[Au14(PPh3)8(NO3)4]: an example of a new class of Au(NO3)-ligated superatom complexes. *Angewandte Chemie - International Edition*, **2013**, 52, 3529-32	16.4	78
253	High throughput in-silico screening against flexible protein receptors. *Journal of Cheminformatics*, **2010**, 2,	8.6	78

252	Theoretical description of the electrical conduction in atomic and molecular junctions. *Nanotechnology*, **2003**, 14, R29-R38	3.4	76
251	Conductance Photoswitching of Metal-Organic Frameworks with Embedded Spiropyran. *Angewandte Chemie - International Edition*, **2019**, 58, 1193-1197	16.4	74
250	Chiral Porous Metacrystals: Employing Liquid-Phase Epitaxy to Assemble Enantiopure Metal-Organic Nanoclusters into Molecular Framework Pores. *ACS Nano*, **2016**, 10, 977-83	16.7	71
249	Photoconductivity in Metal-Organic Framework (MOF) Thin Films. *Angewandte Chemie - International Edition*, **2019**, 58, 9590-9595	16.4	68
248	Nonadiabatic wave packet dynamics on the coupled / electronic states of NO2 based on new ab initio potential energy surfaces. *Chemical Physics*, **2000**, 259, 211-226	2.3	67
247	Branched DNA that forms a solid at 95 °C. *Angewandte Chemie - International Edition*, **2011**, 50, 3227-31	16.4	63
246	Comparison of stochastic optimization methods for receptor□gand docking. *Chemical Physics Letters*, **2002**, 362, 271-277	2.5	63
245	Molecular Origin of the Charge Carrier Mobility in Small Molecule Organic Semiconductors. *Advanced Functional Materials*, **2016**, 26, 5757-5763	15.6	62
244	Visible Light [2 + 2] Cycloadditions for Reversible Polymer Ligation. *Macromolecules*, **2018**, 51, 3802-3807	5.5	61
243	Energy landscape paving simulations of the trp-cage protein. *Journal of Chemical Physics*, **2005**, 122, 194711	3.1	61
242	Toward Design of Novel Materials for Organic Electronics. *Advanced Materials*, **2019**, 31, e1808256	24	60
241	Variable-temperature measurements of the single-molecule conductance of double-stranded DNA. *Angewandte Chemie - International Edition*, **2006**, 45, 5499-502	16.4	60
240	Two base pair duplexes suffice to build a novel material. *ChemBioChem*, **2009**, 10, 1335-9	3.8	58
239	Basin hopping simulations for all-atom protein folding. *Journal of Chemical Physics*, **2006**, 124, 044515	3.9	57
238	Photochemistry in Confined Environments for Single-Chain Nanoparticle Design. *Journal of the American Chemical Society*, **2018**, 140, 9551-9557	16.4	57
237	Non-linear transport through a molecular nanojunction. *Europhysics Letters*, **2002**, 57, 571-577	1.6	56
236	Constrained Synthesis and Organization of Catalytically Active Metal Nanoparticles by Self-Assembled Protein Templates. *Advanced Materials*, **2009**, 21, 3515-3519	24	55
235	An all-atom force field for tertiary structure prediction of helical proteins. *Biophysical Journal*, **2004**, 87, 3100-9	2.9	54

234	Differential hERG ion channel activity of ultrasmall gold nanoparticles. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 8004-9	11.5	53
233	Folding and self-assembly of the TatA translocation pore based on a charge zipper mechanism. *Cell*, **2013**, 152, 316-26	56.2	52
232	Experimental and theoretical investigations of the electronic band structure of metal-organic frameworks of HKUST-1 type. *Applied Physics Letters*, **2015**, 107, 183301	3.4	52
231	Post-synthetic modification of epitaxially grown, highly oriented functionalized MOF thin films. *Chemical Communications*, **2011**, 47, 11210-2	5.8	52
230	Highly Selective Dispersion of Single-Walled Carbon Nanotubes via Polymer Wrapping: A Combinatorial Study via Modular Conjugation. *ACS Macro Letters*, **2014**, 3, 10-15	6.6	51
229	Nasal embryonic LHRH factor (NELF) mutations in patients with normosmic hypogonadotropic hypogonadism and Kallmann syndrome. *Fertility and Sterility*, **2011**, 95, 1613-20.e1-7	4.8	50
228	Spiral states in the square-lattice Hubbard model. *Physical Review B*, **1991**, 43, 8775-8778	3.3	49
227	Frustration-induced Raman scattering in CuGeO3. *Physical Review B*, **1996**, 54, R9635-R9638	3.3	48
226	Superexchange Charge Transport in Loaded Metal Organic Frameworks. *ACS Nano*, **2016**, 10, 7085-93	16.7	48
225	Modeling disordered morphologies in organic semiconductors. *Journal of Computational Chemistry*, **2013**, 34, 2716-25	3.5	47
224	Host dependence of the electron affinity of molecular dopants. *Materials Horizons*, **2019**, 6, 107-114	14.4	44
223	An evolutionary strategy for all-atom folding of the 60-amino-acid bacterial ribosomal protein l20. *Biophysical Journal*, **2006**, 90, 4273-80	2.9	44
222	Six hydrophobins are involved in hydrophobin rodlet formation in Aspergillus nidulans and contribute to hydrophobicity of the spore surface. *PLoS ONE*, **2014**, 9, e94546	3.7	44
221	In silico discovery of a compound with nanomolar affinity to antithrombin causing partial activation and increased heparin affinity. *Journal of Medicinal Chemistry*, **2012**, 55, 6403-12	8.3	43
220	Controlling Chain Coupling and Single-Chain Ligation by Two Colours of Visible Light. *Angewandte Chemie - International Edition*, **2019**, 58, 3604-3609	16.4	43
219	Access to Disparate Soft Matter Materials by Curing with Two Colors of Light. *Advanced Materials*, **2019**, 31, e1807288	24	43
218	Flexible side chain models improve enrichment rates in in silico screening. *Journal of Medicinal Chemistry*, **2008**, 51, 5919-31	8.3	42
217	Charge-switchable molecular magnet and spin blockade of tunneling. *Physical Review B*, **2007**, 75,	3.3	42

216	Built-In Potentials Induced by Molecular Order in Amorphous Organic Thin Films. *ACS Applied Materials & Interfaces*, **2018**, 10, 1881-1887	9.5	40
215	Catalytic subsurface etching of nanoscale channels in graphite. *Nature Communications*, **2013**, 4, 1379	17.4	40
214	Independently switchable atomic quantum transistors by reversible contact reconstruction. *Nano Letters*, **2008**, 8, 4493-7	11.5	39
213	Brillouin□Wigner based multi-reference perturbation theory for electronic correlation effects. *Journal of Chemical Physics*, **1998**, 108, 4714-4724	3.9	39
212	Unstable periodic orbits and the symbolic dynamics of the complex H□non map. *Physical Review A*, **1990**, 42, 4639-4646	2.6	39
211	Ab initio charge-carrier mobility model for amorphous molecular semiconductors. *Physical Review B* , **2016**, 93,	3.3	38
210	Mechanisms of Nanoglass Ultrastability. *ACS Nano*, **2016**, 10, 3241-7	16.7	38
209	Characterizing single chain nanoparticles (SCNPs): a critical survey. *Polymer Chemistry*, **2017**, 8, 5845-5854	4.9	38
208	Receptor flexibility in small-molecule docking calculations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 298-314	7.9	38
207	Metal-Insulator Transition in the Hubbard Model on a Triangular Lattice. *Europhysics Letters*, **1991**, 15, 625-630	1.6	37
206	Free-energy landscape of the villin headpiece in an all-atom force field. *Structure*, **2005**, 13, 661-8	5.2	36
205	Comparison of stochastic optimization methods for all-atom folding of the Trp-Cage protein. *ChemPhysChem*, **2005**, 6, 2640-6	3.2	36
204	Microemulsions: A Landau-Ginzburg theory. *Physical Review Letters*, **1990**, 65, 2736-2739	7.4	36
203	Cloning, functional characterization, and remodeling of K2P3.1 (TASK-1) potassium channels in a porcine model of atrial fibrillation and heart failure. *Heart Rhythm*, **2014**, 11, 1798-805	6.7	35
202	Anisotropic energy transfer in crystalline chromophore assemblies. *Nature Communications*, **2018**, 9, 4332	17.4	35
201	Toward Fast and Accurate Evaluation of Charge On-Site Energies and Transfer Integrals in Supramolecular Architectures Using Linear Constrained Density Functional Theory (CDFT)-Based Methods. *Journal of Chemical Theory and Computation*, **2015**, 11, 2077-86	6.4	34
200	hERG K+ channel-associated cardiac effects of the antidepressant drug desipramine. *Naunyn-Schmiedeberg's Archives of Pharmacology*, **2011**, 383, 119-39	3.4	34
199	Application of the stochastic tunneling method to high throughput database screening. *Chemical Physics Letters*, **2003**, 370, 68-73	2.5	34

198	Macromolecular Superstructures: A Future Beyond Single Chain Nanoparticles. *Israel Journal of Chemistry*, **2020**, 60, 86-99	3.4	33
197	Receptor-specific scoring functions derived from quantum chemical models improve affinity estimates for in-silico drug discovery. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 1264-73	4.2	33
196	In silico folding of a three helix protein and characterization of its free-energy landscape in an all-atom force field. *Physical Review Letters*, **2005**, 94, 018101	7.4	33
195	Scaling behavior of stochastic minimization algorithms in a perfect funnel landscape. *Physical Review E*, **1999**, 59, 938-941	2.4	33
194	QM/QM approach to model energy disorder in amorphous organic semiconductors. *Journal of Chemical Theory and Computation*, **2015**, 11, 560-7	6.4	32
193	Selective dispersion of large-diameter semiconducting single-walled carbon nanotubes with pyridine-containing copolymers. *Small*, **2014**, 10, 360-7	11	32
192	Structural model of the gas vesicle protein GvpA and analysis of GvpA mutants in vivo. *Molecular Microbiology*, **2011**, 81, 56-68	4.1	32
191	Charge Transport by Superexchange in Molecular Host-Guest Systems. *Physical Review Letters*, **2016**, 117, 276803	7.4	32
190	Bunching and Immobilization of Ionic Liquids in Nanoporous Metal-Organic Framework. *Nano Letters*, **2019**, 19, 2114-2120	11.5	31
189	Wavelength-Dependent Stiffening of Hydrogel Matrices via Redshifted [2+2] Photocycloadditions. *Advanced Functional Materials*, **2020**, 30, 1908171	15.6	31
188	Periodic orbits in the dissipative standard map. *Physical Review A*, **1991**, 43, 6550-6557	2.6	31
187	(4,4′)-Bipyridine in vacuo and in solvents: a quantum chemical study of a prototypical floppy molecule from a molecular transport perspective. *Physical Chemistry Chemical Physics*, **2013**, 15, 1918-28	3.6	30
186	Cardiac expression and atrial fibrillation-associated remodeling of K2P2.1 (TREK-1) K+ channels in a porcine model. *Life Sciences*, **2014**, 97, 107-15	6.8	30
185	Mirror images as naturally competing conformations in protein folding. *Journal of Physical Chemistry B*, **2012**, 116, 6880-8	3.4	30
184	All-atom folding of the three-helix HIV accessory protein with an adaptive parallel tempering method. *Proteins: Structure, Function and Bioinformatics*, **2004**, 57, 792-8	4.2	30
183	Full quantum treatment of charge dynamics in amorphous molecular semiconductors. *Physical Review B*, **2018**, 97,	3.3	29
182	7-Alkyl-3-benzylcoumarins: a versatile scaffold for the development of potent and selective cannabinoid receptor agonists and antagonists. *Journal of Medicinal Chemistry*, **2012**, 55, 7967-77	8.3	28
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180	Engineering hydrophobin DewA to generate surfaces that enhance adhesion of human but not bacterial cells. *Acta Biomaterialia*, **2012**, 8, 1037-47	10.8	28
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177	Tailoring the Mechanical Properties of 3D Microstructures Using Visible Light Post-Manufacturing. *Advanced Materials*, **2019**, 31, e1901269	24	27
176	A de novo strategy for predictive crystal engineering to tune excitonic coupling. *Nature Communications*, **2019**, 10, 2048	17.4	27
175	Diameter sorting of carbon nanotubes by gradient centrifugation: role of endohedral water. *Physica Status Solidi (B): Basic Research*, **2007**, 244, 3896-3900	1.3	27
174	Predictive in silico all-atom folding of a four-helix protein with a free-energy model. *Journal of the American Chemical Society*, **2004**, 126, 16736-7	16.4	27
173	Basis set reduction in Hilbert space. *Physical Review Letters*, **1992**, 69, 800-803	7.4	27
172	Spin-crossover and massive anisotropy switching of 5d transition metal atoms on graphene nanoflakes. *Nano Letters*, **2014**, 14, 3364-8	11.5	26
171	Multilevel atomic-scale transistors based on metallic quantum point contacts. *Advanced Materials*, **2010**, 22, 2033-6	24	26
170	Effects of energy correlations and superexchange on charge transport and exciton formation in amorphous molecular semiconductors: An ab initio study. *Physical Review B*, **2017**, 95,	3.3	25
169	Generalized effective-medium model for the carrier mobility in amorphous organic semiconductors. *Physical Review B*, **2015**, 91,	3.3	25
168	Modelling proteins: conformational sampling and reconstruction of folding kinetics. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2011**, 1814, 977-1000	4	25
167	All-atom folding of the trp-cage protein with an adpative parallel tempering method. *Europhysics Letters*, **2004**, 67, 307-313	1.6	25
166	Multireference Brillouin-Wigner Coupled Cluster Singles and Doubles (MRBWCCSD) and Multireference Doubles Configuration Interaction (MRD-CI) Calculations for the Bergman Cyclization Reaction. *Collection of Czechoslovak Chemical Communications*, **2003**, 68, 2309-2321		24
165	Rational In Silico Design of an Organic Semiconductor with Improved Electron Mobility. *Advanced Materials*, **2017**, 29, 1703505	24	23
164	Disorder compensation controls doping efficiency in organic semiconductors. *Nature Communications*, **2019**, 10, 4547	17.4	23
163	Loading of ionic compounds into metal-organic frameworks: a joint theoretical and experimental study for the case of La□+. *Physical Chemistry Chemical Physics*, **2014**, 16, 17918-23	3.6	23

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160	Contemporary Photoligation Chemistry: The Visible Light Challenge. *Chemistry - A European Journal* , **2019**, 25, 3700-3709	4.8	23
159	Bi□□nanoparticles encapsulated in surface mounted metal-organic framework thin films. *Nanoscale*, **2016**, 8, 6468-72	7.7	22
158	Loading of Two Related Metal-Organic Frameworks (MOFs), [Cu2(bdc)2(dabco)] and [Cu2(ndc)2(dabco)], with Ferrocene. *Polymers*, **2011**, 3, 1565-1574	4.5	22
157	Preselectable integer quantum conductance of electrochemically fabricated silver point contacts. *Applied Physics Letters*, **2008**, 93, 043103	3.4	22
156	Green light triggered [2+2] cycloaddition of halochromic styrylquinoxaline-controlling photoreactivity by pH. *Nature Communications*, **2020**, 11, 4193	17.4	22
155	Ultrarobust Thin-Film Devices from Self-Assembled Metal-Terpyridine Oligomers. *Advanced Materials*, **2016**, 28, 3473-80	24	21
154	SIMONA 1.0: an efficient and versatile framework for stochastic simulations of molecular and nanoscale systems. *Journal of Computational Chemistry*, **2012**, 33, 2602-13	3.5	21
153	A free-energy approach for all-atom protein simulation. *Biophysical Journal*, **2009**, 96, 3483-94	2.9	21
152	Influence of Meso and Nanoscale Structure on the Properties of Highly Efficient Small Molecule Solar Cells. *Advanced Energy Materials*, **2016**, 6, 1501280	21.8	21
151	Modelling of reversible single chain polymer self-assembly: from the polymer towards the protein limit. *Chemical Communications*, **2015**, 51, 6002-5	5.8	20
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149	Optimization methods for virtual screening on novel computational architectures. *Current Computer-Aided Drug Design*, **2011**, 7, 44-52	1.4	20
148	Accurate multireference calculations of the electron affinity of NO, BO and O2. *Chemical Physics Letters*, **2003**, 370, 478-484	2.5	20
147	Designing Molecular Printboards: A Photolithographic Platform for Recodable Surfaces. *Chemistry - A European Journal*, **2015**, 21, 13186-90	4.8	19
146	Exploration of the free-energy surface of a three-helix peptide with stochastic optimization methods. *International Journal of Quantum Chemistry*, **2004**, 99, 854-863	2.1	19
145	Investigation of a Kubo-formula-based approach to estimate DNA conductance in an atomistic model. *European Physical Journal E*, **2005**, 18, 437-45	1.5	19

144	Influence of endohedral water on diameter sorting of single-walled carbon nanotubes by density gradient centrifugation. *Physical Chemistry Chemical Physics*, **2010**, 12, 902-8	3.6	18
143	Interactions of hydrophobic and hydrophilic self-assembled monolayers with water as probed by sum-frequency-generation spectroscopy. *Chemical Physics Letters*, **2010**, 494, 193-197	2.5	18
142	Effects of molecular motion on charge transfer/transport through DNA duplexes with and without base pair mismatch. *Molecular Simulation*, **2006**, 32, 759-764	2	18
141	Improved implementation and application of the individually selecting configuration interaction method. *Journal of Chemical Physics*, **2005**, 122, 024110	3.9	18
140	Tuning Optical Properties by Controlled Aggregation: Electroluminescence Assisted by Thermally-Activated Delayed Fluorescence from Thin Films of Crystalline Chromophores. *Chemistry - A European Journal*, **2020**, 26, 17016-17020	4.8	18
139	Lichtinduziertes Schalten der Leitfähigkeit von MOFs mit eingelagertem Spiropyran. *Angewandte Chemie*, **2019**, 131, 1205-1210	3.6	18
138	Binding patterns of homo-peptides on bare magnetic nanoparticles: insights into environmental dependence. *Scientific Reports*, **2017**, 7, 14047	4.9	17
137	Machine learning of correlated dihedral potentials for atomistic molecular force fields. *Scientific Reports*, **2018**, 8, 2559	4.9	17
136	Band-gap engineering with a twist: Formation of intercalant superlattices in twisted graphene bilayers. *Physical Review B*, **2015**, 91,	3.3	17
135	Protein structure prediction by all-atom free-energy refinement. *BMC Structural Biology*, **2007**, 7, 12	2.7	17
134	Interaction-induced collapse of a section of the Fermi sea in the zigzag Hubbard ladder. *Physical Review Letters*, **2002**, 88, 217203	7.4	17
133	Disorder induced quantum phase transition in random-exchange spin-1/2 chains. *Physical Review Letters*, **2002**, 89, 127202	7.4	17
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131	Wavelength-gated photoreversible polymerization and topology control. *Chemical Science*, **2020**, 11, 2834-2842	9.4	15
130	Ligand-lipid and ligand-core affinity control the interaction of gold nanoparticles with artificial lipid bilayers and cell membranes. *Nanomedicine: Nanotechnology, Biology, and Medicine*, **2016**, 12, 1409-19	6	15
129	Modeling loop backbone flexibility in receptor-ligand docking simulations. *Journal of Computational Chemistry*, **2012**, 33, 2504-15	3.5	14
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125	Triplet exciton diffusion in metalorganic phosphorescent host-guest systems from first principles. *Physical Review B*, **2019**, 99,	3.3	12
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121	Breakdown of the Luttinger sum rule at the Mott-Hubbard transition in the one-dimensional t 1 - t 2 Hubbard model. *Europhysics Letters*, **2005**, 69, 616-622	1.6	12
120	Designable electron transport features in one-dimensional arrays of metallic nanoparticles: Monte Carlo study of the relation between shape and transport. *Physical Review B*, **2005**, 72,	3.3	12
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108	A Roadmap for Transforming Research to Invent the Batteries of the Future Designed within the European Large Scale Research Initiative BATTERY 2030+. *Advanced Energy Materials*,2102785	21.8	10
107	Wavelength-Selective Softening of Hydrogel Networks. *Advanced Materials*, **2021**, 33, e2102184	24	10
106	Generalized Born implicit solvent models for small molecule hydration free energies. *Physical Chemistry Chemical Physics*, **2017**, 19, 1677-1685	3.6	9
105	26-4: Computer-Aided Optimization of Multilayer OLED Devices. *Digest of Technical Papers SID International Symposium*, **2018**, 49, 340-342	0.5	9
104	A fluorescence polarization assay for the experimental validation of an in silico model of the chemokine CXCL8 binding to receptor-derived peptides. *Physical Chemistry Chemical Physics*, **2014**, 16, 8036-43	3.6	9
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96	Action Plots in Action: In-Depth Insights into Photochemical Reactivity. *Journal of the American Chemical Society*, **2021**,	16.4	9
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