Sabre Kais

List of Publications by Citations

242 papers	4,630 citations	36 h-index	55 g-index
256 ext. papers	5,427 ext. citations	4 avg, IF	6.02 L-index

#	Paper	IF	Citations
242	Revealing the role of organic cations in hybrid halide perovskite CH3NH3PbI3. *Nature Communications*, **2015**, 6, 7026	17.4	489
241	Manipulation of molecules with electromagnetic fields. *Molecular Physics*, **2013**, 111, 1648-1682	1.7	192
240	Theoretical limits of photovoltaics efficiency and possible improvements by intuitive approaches learned from photosynthesis and quantum coherence. *Renewable and Sustainable Energy Reviews*, **2015**, 43, 1073-1089	16.2	112
239	Modified scaled hierarchical equation of motion approach for the study of quantum coherence in photosynthetic complexes. *Journal of Physical Chemistry B*, **2011**, 115, 1531-7	3.4	110
238	Quantum algorithm for obtaining the energy spectrum of molecular systems. *Physical Chemistry Chemical Physics*, **2008**, 10, 5388-93	3.6	83
237	Entanglement as measure of electron-electron correlation in quantum chemistry calculations. *Chemical Physics Letters*, **2005**, 413, 1-5	2.5	82
236	Hydrogen Bonding and Stability of Hybrid Organic-Inorganic Perovskites. *ChemSusChem*, **2016**, 9, 2648-2655	8.5	80
235	Cation Effect on Hot Carrier Cooling in Halide Perovskite Materials. *Journal of Physical Chemistry Letters*, **2017**, 8, 4439-4445	6.4	71
234	Entropic uncertainty relations for Markovian and non-Markovian processes under a structured bosonic reservoir. *Scientific Reports*, **2017**, 7, 1066	4.9	58
233	Tuning the entanglement for a one-dimensional magnetic system with anisotropic coupling and impurities. *Physical Review A*, **2003**, 67,	2.6	58
232	Enhancing the carrier thermalization time in organometallic perovskites by halide mixing. *Physical Chemistry Chemical Physics*, **2016**, 18, 5219-31	3.6	55
231	Quantum machine learning for electronic structure calculations. *Nature Communications*, **2018**, 9, 4195	17.4	55
230	Experimental realization of quantum algorithm for solving linear systems of equations. *Physical Review A*, **2014**, 89,	2.6	53
229	Quantum algorithm and circuit design solving the Poisson equation. *New Journal of Physics*, **2013**, 15, 013021	2.9	51
228	Coherent states for the Morse oscillator. *Physical Review A*, **1990**, 41, 2301-2305	2.6	51
227	Dimensional interpolation of hard sphere virial coefficients. *Journal of Chemical Physics*, **1991**, 95, 4525-4544	3.9	46
226	Finite size scaling for the atomic Shannon-information entropy. *Journal of Chemical Physics*, **2004**, 121, 5611-7	3.9	45

225	Entanglement and electron correlation in quantum chemistry calculations. *Journal of Modern Optics* , **2006**, 53, 2543-2558	1.1	43
224	Study of phase changes of the water octamer using parallel tempering and multihistogram methods. *Journal of Chemical Physics*, **2001**, 115, 2621-2628	3.9	43
223	Quantum criticality and stability of three-body Coulomb systems. *Physical Review A*, **2000**, 62,	2.6	43
222	Quantum Annealing for Prime Factorization. *Scientific Reports*, **2018**, 8, 17667	4.9	43
221	Delocalized quantum states enhance photocell efficiency. *Physical Chemistry Chemical Physics*, **2015** , 17, 5743-50	3.6	42
220	Implementation of quantum logic gates using polar molecules in pendular states. *Journal of Chemical Physics*, **2013**, 138, 024104	3.9	42
219	Discontinuity of Shannon information entropy for two-electron atoms. *Chemical Physics*, **2005**, 309, 127-131	1.3	42
218	Electronic Structure Calculations and the Ising Hamiltonian. *Journal of Physical Chemistry B*, **2018**, 122, 3384-3395	3.4	42
217	Entanglement of polar symmetric top molecules as candidate qubits. *Journal of Chemical Physics*, **2011**, 135, 154102	3.9	40
216	Electronic Structure Critical Parameters From Finite-Size Scaling. *Physical Review Letters*, **1997**, 79, 3142-3145	7.4	40
215	Correlated Protein Environments Drive Quantum Coherence Lifetimes in Photosynthetic Pigment-Protein Complexes. *CheM*, **2018**, 4, 138-149	16.2	39
214	Effects of Hawking Radiation on the Entropic Uncertainty in a Schwarzschild Space-Time. *Annalen Der Physik*, **2018**, 530, 1800080	2.6	39
213	Entanglement of polar molecules in pendular states. *Journal of Chemical Physics*, **2011**, 134, 124107	3.9	39
212	Finite-Size Scaling for Atomic and Molecular Systems. *Advances in Chemical Physics*, **2003**, 1-99		39
211	Decomposition of unitary matrices for finding quantum circuits: application to molecular Hamiltonians. *Journal of Chemical Physics*, **2011**, 134, 144112	3.9	37
210	Electronic Structure Critical Parameters For the Lithium Isoelectronic Series. *Physical Review Letters* , **1998**, 80, 5293-5296	7.4	37
209	Critical Phenomena for Electronic Structure at the Large-Dimension Limit. *Physical Review Letters*, **1996**, 77, 466-469	7.4	37
208	Domain Walls Conductivity in Hybrid Organometallic Perovskites and Their Essential Role in CH3NH3PbI3 Solar Cell High Performance. *Scientific Reports*, **2015**, 5, 11467	4.9	36

207	Entanglement evolution of one-dimensional spin systems in external magnetic fields. *Physical Review A*, **2006**, 73,	2.6	36
206	Large-Z and -N dependence of atomic energies from renormalization of the large-dimension limit. *International Journal of Quantum Chemistry*, **1994**, 49, 657-674	2.1	36
205	On the interactions between atmospheric radicals and cloud droplets: a molecular picture of the interface. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 9686-90	11.5	35
204	Quantum critical phenomena and stability of atomic and molecular ions. *International Reviews in Physical Chemistry*, **2000**, 19, 97-121	7	35
203	Pivot method for global optimization: a study of water clusters (H2O)N with 2?N?33. *Chemical Physics Letters*, **1999**, 305, 433-438	2.5	35
202	Enhancing Intrinsic Stability of Hybrid Perovskite Solar Cell by Strong, yet Balanced, Electronic Coupling. *Scientific Reports*, **2016**, 6, 30305	4.9	33
201	Prospects for quantum computing with an array of ultracold polar paramagnetic molecules. *Journal of Chemical Physics*, **2016**, 144, 094301	3.9	33
200	Reduced work function of graphene by metal adatoms. *Applied Surface Science*, **2017**, 394, 98-107	6.7	32
199	Degree Distribution in Quantum Walks on Complex Networks. *Physical Review X*, **2013**, 3,	9.1	32
198	Quantum coherence and entanglement in the avian compass. *Physical Review E*, **2013**, 87, 062704	2.4	32
197	Comparison study of pivot methods for global optimization. *Journal of Chemical Physics*, **1997**, 106, 7170-7177	3.9	32
196	Finite-size scaling approach for the Schr□dinger equation. *Physical Review A*, **1998**, 57, R1481-R1484	2.6	32
195	Large order dimensional perturbation theory for complex energy eigenvalues. *Journal of Chemical Physics*, **1993**, 99, 7739-7747	3.9	32
194	Multipartite quantum entanglement evolution in photosynthetic complexes. *Journal of Chemical Physics*, **2012**, 137, 074112	3.9	30
193	Critical nuclear charges for N-electron atoms. *International Journal of Quantum Chemistry*, **1999**, 75, 533-542	2.1	30
192	Infrared-dressed entanglement of cold open-shell polar molecules for universal matchgate quantum computing. *New Journal of Physics*, **2014**, 16, 075001	2.9	29
191	Entanglement of formation for one-dimensional magnetic systems with defects. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2004**, 322, 137-145	2.3	29
190	An efficient descriptor model for designing materials for solar cells. *Npj Computational Materials*, **2015**, 1,	10.9	28

189	Group leaders optimization algorithm. *Molecular Physics*, **2011**, 109, 761-772	1.7	28
188	Entanglement, Electron Correlation, and Density Matrices. *Advances in Chemical Physics*, **2007**, 493-535		27
187	Hydrogen bonding and orientation effects on the accommodation of methylamine at the air-water interface. *Journal of Chemical Physics*, **2016**, 144, 214701	3.9	27
186	Elucidation of near-resonance vibronic coherence lifetimes by nonadiabatic electronic-vibrational state character mixing. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 18263-18268	11.5	26
185	Ground-state stability and criticality of two-electron atoms with screened Coulomb potentials using the B-splines basis set. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2012**, 45, 235003	1.3	25
184	Pivot method for global optimization. *Physical Review E*, **1997**, 55, 1162-1165	2.4	25
183	A quantum algorithm for evolving open quantum dynamics on quantum computing devices. *Scientific Reports*, **2020**, 10, 3301	4.9	24
182	Finite-size scaling for critical conditions for stable quadrupole-bound anions. *Journal of Chemical Physics*, **2004**, 120, 8412-9	3.9	24
181	Interfaces Select Specific Stereochemical Conformations: The Isomerization of Glyoxal at the Liquid Water Interface. *Journal of the American Chemical Society*, **2017**, 139, 27-30	16.4	23
180	Finite size scaling for critical conditions for stable dipole-bound anions. *Chemical Physics Letters*, **2003**, 372, 205-209	2.5	23
179	The 1/Z expansion and renormalization of the large-dimension limit for many-electron atoms. *Journal of Chemical Physics*, **1994**, 100, 4367-4376	3.9	23
178	Entanglement, Berry phases, and level crossings for the atomic Breit-Rabi Hamiltonian. *Physical Review A*, **2008**, 78,	2.6	22
177	Crossover phenomena and resonances in quantum systems. *Physical Review A*, **2001**, 64,	2.6	22
176	Probing entropic uncertainty relations under a two-atom system coupled with structured bosonic reservoirs. *Quantum Information Processing*, **2018**, 17, 1	1.6	22
175	The radical pair mechanism and the avian chemical compass: Quantum coherence and entanglement. *International Journal of Quantum Chemistry*, **2015**, 115, 1327-1341	2.1	21
174	Multicritical phenomena for the hydrogen molecule at the large-dimension limit. *Chemical Physics Letters*, **1996**, 260, 302-308	2.5	21
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172	Quantum computing methods for electronic states of the water molecule. *Molecular Physics*, **2019**, 117, 2069-2082	1.7	20

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169	Population and coherence dynamics in light harvesting complex II (LH2). *Journal of Chemical Physics* , **2012**, 137, 084110	3.9	20
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166	Quantum circuit design for solving linear systems of equations. *Molecular Physics*, **2012**, 110, 1675-1680	1.7	19
165	Phase transitions for N-electron atoms at the large-dimension limit. *Physical Review A*, **1997**, 55, 238-247	2.6	19
164	Generalized Remote Preparation of Arbitrary m-qubit Entangled States via Genuine Entanglements. *Entropy*, **2015**, 17, 1755-1774	2.8	18
163	Dynamics of entanglement in a two-dimensional spin system. *Physical Review A*, **2011**, 83,	2.6	18
162	New stable multiply charged negative atomic ions in linearly polarized superintense laser fields. *Journal of Chemical Physics*, **2006**, 124, 201108	3.9	18
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160	Qudits and High-Dimensional Quantum Computing. *Frontiers in Physics*, **2020**, 8,	3.9	18
159	Tuning the Stereoselectivity and Solvation Selectivity at Interfacial and Bulk Environments by Changing Solvent Polarity: Isomerization of Glyoxal in Different Solvent Environments. *Journal of the American Chemical Society*, **2018**, 140, 5535-5543	16.4	17
158	Communications: Entanglement switch for dipole arrays. *Journal of Chemical Physics*, **2010**, 132, 121104	3.9	17
157	The repulsive Coulomb barrier along a dissociation path of the BeC(2-)(4) dianion. *Journal of the American Chemical Society*, **2002**, 124, 11723-9	16.4	17
156	Exact calculation of entanglement in a 19-site two-dimensional spin system. *Physical Review A*, **2010** , 81,	2.6	16
155	Entanglement dynamics of one-dimensional driven spin systems in time-varying magnetic fields. *Physical Review A*, **2011**, 84,	2.6	16
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148	Quantum teleportation in one-dimensional quantum dots system. *Chemical Physics Letters*, **2006**, 421, 338-342	2.5	15
147	Study of electronic structure and dynamics of interacting free radicals influenced by water. *Journal of Chemical Physics*, **2009**, 130, 124312	3.9	14
146	Gas-Phase Reactions of Fe(CH2O)+ and Fe(CH2S)+ with Small Alkanes: An Experimental and Theoretical Study. *Journal of the American Chemical Society*, **1997**, 119, 12879-12888	16.4	14
145	A new approach to global minimization. *Journal of Computational Chemistry*, **1997**, 18, 594-599	3.5	14
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139	Efficient Remote Preparation of Four-Qubit Cluster-Type Entangled States with Multi-Party Over Partially Entangled Channels. *International Journal of Theoretical Physics*, **2016**, 55, 3454-3466	1.1	14
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137	Tuning entanglement and ergodicity in two-dimensional spin systems using impurities and anisotropy. *Physical Review A*, **2012**, 85,	2.6	12
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133	A universal quantum circuit scheme for finding complex eigenvalues. *Quantum Information Processing*, **2014**, 13, 333-353	1.6	11
132	The interference effect of laser-assisted bremsstrahlung emission in Coulomb fields of two nuclei. *Journal of Applied Physics*, **2013**, 114, 124904	2.5	11
131	Neuroreceptor activation by vibration-assisted tunneling. *Scientific Reports*, **2015**, 5, 9990	4.9	11
130	Time-dependent density functional theory of coupled electronic lattice motion in quasi-two-dimensional crystals. *Physical Review B*, **2014**, 89,	3.3	11
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126	Experimental evaluation of the generalized vibrational theory of G protein-coupled receptor activation. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 5595-5600	11.5	10
125	Role of Water on the Rotational Dynamics of the Organic Methylammonium Cation: A First Principles Analysis. *Scientific Reports*, **2019**, 9, 668	4.9	10
124	Dark states and delocalization: Competing effects of quantum coherence on the efficiency of light harvesting systems. *Journal of Chemical Physics*, **2018**, 148, 064304	3.9	10
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118	Finite size scaling for critical parameters of simple diatomic molecules. *Molecular Physics*, **2000**, 98, 1485-1493	1.7	10

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115	Direct application of the phase estimation algorithm to find the eigenvalues of the Hamiltonians. *Chemical Physics*, **2018**, 514, 87-94	2.3	9
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98	Electronic isomerism: symmetry breaking and electronic phase diagrams for diatomic molecules at the large-dimension limit. *ChemPhysChem*, **2001**, 2, 434-42	3.2	7
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94	Enhancement of Photovoltaic Current through Dark States in Donor-Acceptor Pairs of Tungsten-Based Transition Metal Di-Chalcogenides. *Advanced Functional Materials*, **2021**, 31, 2100387	15.6	7
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92	Simulated two-dimensional electronic spectroscopy of the eight-bacteriochlorophyll FMO complex. *Journal of Chemical Physics*, **2014**, 141, 234105	3.9	6
91	Critical conditions for stable dipole-bound dianions. *Journal of Chemical Physics*, **2008**, 128, 044307	3.9	6
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61	On the divergence of gradient expansions for kinetic energy functionals in the potential functional theory. *Journal of Physics A: Mathematical and Theoretical*, **2016**, 49, 285202	2	3
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