Libor Veis

List of Publications by Year in Descending Order

35 papers	861 citations	15 h-index	28 g-index
40 ext. papers	1,245 ext. citations	7.6 avg, IF	4.49 L-index

#	Paper	IF	Citations
35	Efficient Adiabatic Connection Approach for Strongly Correlated Systems: Application to Singlet-Triplet Gaps of Biradicals.. *Journal of Physical Chemistry Letters*, **2022**, 4570-4578	6.4	1
34	Density Matrix Renormalization Group with Dynamical Correlation via Adiabatic Connection. *Journal of Chemical Theory and Computation*, **2021**,	6.4	7
33	Variational quantum eigensolver for approximate diagonalization of downfolded Hamiltonians using generalized unitary coupled cluster ansatz. *Quantum Science and Technology*, **2021**, 6, 034008	5.5	7
32	On-Surface Synthesis and Characterization of [7]Triangulene Quantum Ring. *Nano Letters*, **2021**, 21, 861-867	11.5	23
31	Unravelling the Open-Shell Character of Peripentacene on Au(111). *Journal of Physical Chemistry Letters*, **2021**, 12, 330-336	6.4	12
30	On-Surface Strain-Driven Synthesis of Nonalternant Non-Benzenoid Aromatic Compounds Containing Four- to Eight-Membered Rings. *Journal of the American Chemical Society*, **2021**, 143, 14694-14702	16.4	2
29	Machine Learning-Assisted Selection of Active Spaces for Strongly Correlated Transition Metal Systems. *Journal of Chemical Theory and Computation*, **2021**, 17, 6053-6072	6.4	9
28	DMRG on Top of Plane-Wave Kohn-Sham Orbitals: A Case Study of Defected Boron Nitride. *Journal of Chemical Theory and Computation*, **2021**, 17, 1143-1154	6.4	9
27	Massively parallel quantum chemical density matrix renormalization group method. *Journal of Computational Chemistry*, **2021**, 42, 534-544	3.5	10
26	Toward DMRG-tailored coupled cluster method in the 4c-relativistic domain. *Journal of Chemical Physics*, **2020**, 152, 174107	3.9	8
25	Near-Linear Scaling in DMRG-Based Tailored Coupled Clusters: An Implementation of DLPNO-TCCSD and DLPNO-TCCSD(T). *Journal of Chemical Theory and Computation*, **2020**, 16, 3028-3040	6.4	7
24	Solving Coupled Cluster Equations by the Newton Krylov Method. *Frontiers in Chemistry*, **2020**, 8, 590184	5	4
23	Ground state of the Fe(ii)-porphyrin model system corresponds to quintet: a DFT and DMRG-based tailored CC study. *Physical Chemistry Chemical Physics*, **2020**, 22, 17033-17037	3.6	10
22	On-Surface Hydrogenation of Buckybowls: From Curved Aromatic Molecules to Planar Non-Kekul Aromatic Hydrocarbons. *ACS Nano*, **2020**,	16.7	9
21	Quantum Chemistry in the Age of Quantum Computing. *Chemical Reviews*, **2019**, 119, 10856-10915	68.1	288
20	Toward the efficient local tailored coupled cluster approximation and the peculiar case of oxo-Mn(Salen). *Journal of Chemical Physics*, **2019**, 151, 084112	3.9	11
19	Quantum information-based analysis of electron-deficient bonds. *Journal of Chemical Physics*, **2019**, 150, 204117	3.9	5

18	Low-depth circuit ansatz for preparing correlated fermionic states on a quantum computer. *Quantum Science and Technology*, **2019**, 4, 045005	5.5	36
17	Capturing the Dynamic Correlation for Arbitrary Spin-Symmetry CASSCF Reference with Adiabatic Connection Approaches: Insights into the Electronic Structure of the Tetramethyleneethane Diradical. *Journal of Physical Chemistry Letters*, **2019**, 10, 4668-4674	6.4	9
16	Numerical and Theoretical Aspects of the DMRG-TCC Method Exemplified by the Nitrogen Dimer. *Journal of Chemical Theory and Computation*, **2019**, 15, 2206-2220	6.4	25
15	The Intricate Case of Tetramethyleneethane: A Full Configuration Interaction Quantum Monte Carlo Benchmark and Multireference Coupled Cluster Studies. *Journal of Chemical Theory and Computation*, **2018**, 14, 2439-2445	6.4	24
14	An Isolated Molecule of Iron(II) Phthalocyanin Exhibits Quintet Ground-State: A Nexus between Theory and Experiment. *Chemistry - A European Journal*, **2018**, 24, 13413-13417	4.8	7
13	The correlation theory of the chemical bond. *Scientific Reports*, **2017**, 7, 2237	4.9	29
12	Fermionic Orbital Optimization in Tensor Network States. *Physical Review Letters*, **2016**, 117, 210402	7.4	28
11	H□kel-Hubbard-Ohno modeling of □bonds in ethene and ethyne with application to trans-polyacetylene. *Physical Chemistry Chemical Physics*, **2016**, 18, 18835-45	3.6	3
10	Quantum chemistry beyond Born□Oppenheimer approximation on a quantum computer: A simulated phase estimation study. *International Journal of Quantum Chemistry*, **2016**, 116, 1328-1336	2.1	21
9	Coupled Cluster Method with Single and Double Excitations Tailored by Matrix Product State Wave Functions. *Journal of Physical Chemistry Letters*, **2016**, 7, 4072-4078	6.4	59
8	Advanced density matrix renormalization group method for nuclear structure calculations. *Physical Review C*, **2015**, 92,	2.7	18
7	Quantum Computing Approach to Nonrelativistic and Relativistic Molecular Energy Calculations. *Advances in Chemical Physics*, **2014**, 107-136		2
6	Adiabatic state preparation study of methylene. *Journal of Chemical Physics*, **2014**, 140, 214111	3.9	30
5	Relativistic quantum chemistry on quantum computers. *Physical Review A*, **2012**, 85,	2.6	25
4	Quantum computing applied to calculations of molecular energies: CH2 benchmark. *Journal of Chemical Physics*, **2010**, 133, 194106	3.9	41
3	Ab initio calculations on the formation and rearrangement of spiropentane. *Journal of Physical Chemistry A*, **2009**, 113, 10557-63	2.8	24
2	Coupled Cluster Study of Polycyclopentanes: Structure and Properties of C5H2n, n = 0-4. *Collection of Czechoslovak Chemical Communications*, **2008**, 73, 1525-1551		15
1	On-line preconcentration of weak electrolytes by electrokinetic accumulation in CE: experiment and simulation. *Electrophoresis*, **2007**, 28, 1540-7	3.6	33