Venkat Kapil

List of Publications by Year in Descending Order

19 papers	504 citations	12 h-index	19 g-index
19 ext. papers	719 ext. citations	7.1 avg, IF	4.17 L-index

#	Paper	IF	Citations
19	A complete description of thermodynamic stabilities of molecular crystals.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119,	11.5	1
18	General embedded cluster protocol for accurate modeling of oxygen vacancies in metal-oxides.. *Journal of Chemical Physics*, **2022**, 156, 124704	3.9	0
17	Uncertainty estimation for molecular dynamics and sampling. *Journal of Chemical Physics*, **2021**, 154, 074102	3.9	20
16	Simulating the ghost: quantum dynamics of the solvated electron. *Nature Communications*, **2021**, 12, 766	17.4	13
15	Importance of Nuclear Quantum Effects for NMR Crystallography. *Journal of Physical Chemistry Letters*, **2021**, 12, 7701-7707	6.4	5
14	Efficient Quantum Vibrational Spectroscopy of Water with High-Order Path Integrals: From Bulk to Interfaces. *Journal of Physical Chemistry Letters*, **2021**, 12, 9108-9114	6.4	3
13	Inexpensive modeling of quantum dynamics using path integral generalized Langevin equation thermostats. *Journal of Chemical Physics*, **2020**, 152, 124104	3.9	15
12	Accurate Description of Nuclear Quantum Effects with High-Order Perturbed Path Integrals (HOPPI). *Journal of Chemical Theory and Computation*, **2020**, 16, 1128-1135	6.4	6
11	Assessment of Approximate Methods for Anharmonic Free Energies. *Journal of Chemical Theory and Computation*, **2019**, 15, 5845-5857	6.4	19
10	Modeling the Structural and Thermal Properties of Loaded Metal-Organic Frameworks. An Interplay of Quantum and Anharmonic Fluctuations. *Journal of Chemical Theory and Computation*, **2019**, 15, 3237-3249	6.4	14
9	Thermal Engineering of Metal-Organic Frameworks for Adsorption Applications: A Molecular Simulation Perspective. *ACS Applied Materials & Interfaces*, **2019**, 11, 38697-38707	9.5	23
8	Barely porous organic cages for hydrogen isotope separation. *Science*, **2019**, 366, 613-620	33.3	101
7	i-PI 2.0: A universal force engine for advanced molecular simulations. *Computer Physics Communications*, **2019**, 236, 214-223	4.2	118
6	Fine tuning classical and quantum molecular dynamics using a generalized Langevin equation. *Journal of Chemical Physics*, **2018**, 148, 102301	3.9	41
5	Anisotropy of the Proton Momentum Distribution in Water. *Journal of Physical Chemistry B*, **2018**, 122, 6048-6054	3.4	10
4	Hydrogen dynamics in solid formic acid: insights from simulations with quantum colored-noise thermostats. *Journal of Physics: Conference Series*, **2018**, 1055, 012003	0.3	6
3	Sampling free energy surfaces as slices by combining umbrella sampling and metadynamics. *Journal of Computational Chemistry*, **2016**, 37, 1413-24	3.5	27

2	High order path integrals made easy. *Journal of Chemical Physics*, **2016**, 145, 234103	3.9	37
1	Accurate molecular dynamics and nuclear quantum effects at low cost by multiple steps in real and imaginary time: Using density functional theory to accelerate wavefunction methods. *Journal of Chemical Physics*, **2016**, 144, 054111	3.9	45