

# Venkat Kapil

## List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	i-PI 2.0: A universal force engine for advanced molecular simulations. <i>Computer Physics Communications</i> , <b>2019</b> , 236, 214-223	4.2	118
18	Barely porous organic cages for hydrogen isotope separation. <i>Science</i> , <b>2019</b> , 366, 613-620	33.3	101
17	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. <i>Journal of Chemical Physics</i> , <b>2016</b> , 144, 054111	3.9	45
16	Fine tuning classical and quantum molecular dynamics using a generalized Langevin equation. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 102301	3.9	41
15	High order path integrals made easy. <i>Journal of Chemical Physics</i> , <b>2016</b> , 145, 234103	3.9	37
14	Sampling free energy surfaces as slices by combining umbrella sampling and metadynamics. <i>Journal of Computational Chemistry</i> , <b>2016</b> , 37, 1413-24	3.5	27
13	Thermal Engineering of Metal-Organic Frameworks for Adsorption Applications: A Molecular Simulation Perspective. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 38697-38707	9.5	23
12	Uncertainty estimation for molecular dynamics and sampling. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 074102	3.9	20
11	Assessment of Approximate Methods for Anharmonic Free Energies. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 5845-5857	6.4	19
10	Inexpensive modeling of quantum dynamics using path integral generalized Langevin equation thermostats. <i>Journal of Chemical Physics</i> , <b>2020</b> , 152, 124104	3.9	15
9	Modeling the Structural and Thermal Properties of Loaded Metal-Organic Frameworks. An Interplay of Quantum and Anharmonic Fluctuations. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 3237-3249	6.4	14
8	Simulating the ghost: quantum dynamics of the solvated electron. <i>Nature Communications</i> , <b>2021</b> , 12, 766	17.4	13
7	Anisotropy of the Proton Momentum Distribution in Water. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 6048-6054	3.4	10
6	Accurate Description of Nuclear Quantum Effects with High-Order Perturbed Path Integrals (HOPPI). <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 1128-1135	6.4	6
5	Hydrogen dynamics in solid formic acid: insights from simulations with quantum colored-noise thermostats. <i>Journal of Physics: Conference Series</i> , <b>2018</b> , 1055, 012003	0.3	6
4	Importance of Nuclear Quantum Effects for NMR Crystallography. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 7701-7707	6.4	5
3	Efficient Quantum Vibrational Spectroscopy of Water with High-Order Path Integrals: From Bulk to Interfaces. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 9108-9114	6.4	3

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| 2 | A complete description of thermodynamic stabilities of molecular crystals.. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2022</b> , 119, | 11.5 | 1 |
| 1 | General embedded cluster protocol for accurate modeling of oxygen vacancies in metal-oxides.. <i>Journal of Chemical Physics</i> , <b>2022</b> , 156, 124704                            | 3.9  | 0 |