Chang-Yu Hsieh

List of Publications by Year
in descending order

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19	578	623734	888059
papers	citations	14 h-index	17 g-index

21	21	21	404
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Physics of lateral triple quantum-dot molecules with controlled electron numbers. Reports on Progress in Physics, 2012, 75, 114501.	20.1	105
2	A unified stochastic formulation of dissipative quantum dynamics. I. Generalized hierarchical equations. Journal of Chemical Physics, 2018, 148, 014103.	3.0	58
3	Accurate Long-Time Mixed Quantum-Classical Liouville Dynamics via the Transfer Tensor Method. Journal of Physical Chemistry Letters, 2016, 7, 4809-4814.	4.6	49
4	A unified stochastic formulation of dissipative quantum dynamics. II. Beyond linear response of spin baths. Journal of Chemical Physics, 2018, 148, 014104.	3.0	46
5	RetroPrime: A Diverse, plausible and Transformer-based method for Single-Step retrosynthesis predictions. Chemical Engineering Journal, 2021, 420, 129845.	12.7	44
6	Mining Toxicity Information from Large Amounts of Toxicity Data. Journal of Medicinal Chemistry, 2021, 64, 6924-6936.	6.4	39
7	RELATION: A Deep Generative Model for Structure-Based De Novo Drug Design. Journal of Medicinal Chemistry, 2022, 65, 9478-9492.	6.4	36
8	A survey on HHL algorithm: From theory to application in quantum machine learning. Physics Letters, Section A: General, Atomic and Solid State Physics, 2020, 384, 126595.	2.1	35
9	Nonadiabatic Dynamics via the Symmetrical Quasi-Classical Method in the Presence of Anharmonicity. Journal of Physical Chemistry Letters, 2018, 9, 319-326.	4.6	32
10	Knowledge-based BERT: a method to extract molecular features like computational chemists. Briefings in Bioinformatics, 2022, 23, .	6.5	24
11	Neural predictor based quantum architecture search. Machine Learning: Science and Technology, 2021, 2, 045027.	5.0	23
12	Variational Quantum-Neural Hybrid Eigensolver. Physical Review Letters, 2022, 128, 120502.	7.8	20
13	Non-Markovian Noise Characterization with the Transfer Tensor Method. Physical Review Applied, 2020, 13, .	3.8	18
14	Introducing block design in graph neural networks for molecular properties prediction. Chemical Engineering Journal, 2021, 414, 128817.	12.7	17
15	An adaptive graph learning method for automated molecular interactions and properties predictions. Nature Machine Intelligence, 2022, 4, 645-651.	16.0	15
16	Out-of-the-box deep learning prediction of quantum-mechanical partial charges by graph representation and transfer learning. Briefings in Bioinformatics, 2022, 23, .	6.5	7
17	Exploring Low-Toxicity Chemical Space with Deep Learning for Molecular Generation. Journal of Chemical Information and Modeling, 0, , .	5.4	5
18	Resonant transition-based quantum computation. Quantum Information Processing, 2017, 16, 1.	2.2	3

#	Article	IF	Citations
19	Spectral-Transfer-Tensor Method for Characterizing Non-Markovian Noise. Physical Review Applied, 2022, 17, .	3.8	0