Chang-Yu Hsieh

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5383331/publications.pdf

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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	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
2	Knowledge-based BERT: a method to extract molecular features like computational chemists. Briefings in Bioinformatics, 2022, 23, .	6.5	24
3	Variational Quantum-Neural Hybrid Eigensolver. Physical Review Letters, 2022, 128, 120502.	7.8	20
4	Spectral-Transfer-Tensor Method for Characterizing Non-Markovian Noise. Physical Review Applied, 2022, 17, .	3.8	0
5	An adaptive graph learning method for automated molecular interactions and properties predictions. Nature Machine Intelligence, 2022, 4, 645-651.	16.0	15
6	RELATION: A Deep Generative Model for Structure-Based De Novo Drug Design. Journal of Medicinal Chemistry, 2022, 65, 9478-9492.	6.4	36
7	Mining Toxicity Information from Large Amounts of Toxicity Data. Journal of Medicinal Chemistry, 2021, 64, 6924-6936.	6.4	39
8	Introducing block design in graph neural networks for molecular properties prediction. Chemical Engineering Journal, 2021, 414, 128817.	12.7	17
9	Neural predictor based quantum architecture search. Machine Learning: Science and Technology, 2021, 2, 045027.	5.0	23
10	RetroPrime: A Diverse, plausible and Transformer-based method for Single-Step retrosynthesis predictions. Chemical Engineering Journal, 2021, 420, 129845.	12.7	44
11	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
12	Non-Markovian Noise Characterization with the Transfer Tensor Method. Physical Review Applied, 2020, 13, .	3.8	18
13	A unified stochastic formulation of dissipative quantum dynamics. I. Generalized hierarchical equations. Journal of Chemical Physics, 2018, 148, 014103.	3.0	58
14	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
15	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
16	Resonant transition-based quantum computation. Quantum Information Processing, 2017, 16, 1.	2.2	3
17	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
18	Physics of lateral triple quantum-dot molecules with controlled electron numbers. Reports on Progress in Physics, 2012, 75, 114501.	20.1	105

#	Article	IF	Citations
19	Exploring Low-Toxicity Chemical Space with Deep Learning for Molecular Generation. Journal of Chemical Information and Modeling, 0, , .	5.4	5