Constantinos C Pantelides

List of Publications by Year
in descending order

31 papers	2,333 citations	430442 18 h-index	433756 31 g-index
32 all docs	32 docs citations	32 times ranked	1879 citing authors

#	Article	IF	Citations
1	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	0.5	445
2	The Consistent Initialization of Differential-Algebraic Systems. SIAM Journal on Scientific and Statistical Computing, 1988, 9, 213-231.	1.5	408
3	Towards crystal structure prediction of complex organic compounds â€“ a report on the fifth blind test. Acta Crystallographica Section B: Structural Science, 2011, 67, 535-551.	1.8	358
4	Ab initio crystal structure prediction?I. Rigid molecules. Journal of Computational Chemistry, 2005, 26, 304-324.	1.5	128
5	Can the Formation of Pharmaceutical Cocrystals Be Computationally Predicted? 2. Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2009, 5, 1432-1448.	2.3	118
6	Successful prediction of a model pharmaceutical in the fifth blind test of crystal structure prediction. International Journal of Pharmaceutics, 2011, 418, 168-178.	2.6	110
7	An Exact Reformulation Algorithm for Large Nonconvex NLPs Involving Bilinear Terms. Journal of Global Optimization, 2006, 36, 161-189.	1.1	100
8	Optimal Campaign Planning/Scheduling of Multipurpose Batch/Semicontinuous Plants. 1. Mathematical Formulation. Industrial & Engineering Chemistry Research, 1996, 35, 488-509.	1.8	94
9	Optimal Campaign Planning/Scheduling of Multipurpose Batch/Semicontinuous Plants. 2. A Mathematical Decomposition Approach. Industrial & Engineering Chemistry Research, 1996, 35, 510-529.	1.8	78
10	Prediction of the crystal structures of axitinib, a polymorphic pharmaceutical molecule. Chemical Engineering Science, 2015, 121, 60-76.	1.9	64
11	The polymorphs of ROY: application of a systematic crystal structure prediction technique. Acta Crystallographica Section B: Structural Science, 2012, 68, 677-685.	1.8	59
12	Convex Envelopes of Monomials of Odd Degree. Journal of Global Optimization, 2003, 25, 157-168.	1.1	58
13	Efficient Handling of Molecular Flexibility in Ab Initio Generation of Crystal Structures. Journal of Chemical Theory and Computation, 2015, 11, 1957-1969.	2.3	58
14	Optimal long-term campaign planning and design of batch operations. Industrial & Engineering Chemistry Research, 1991, 30, 2308-2321.	1.8	41
15	How many more polymorphs of ROY remain undiscovered. Chemical Science, 2022, 13, 1288-1297.	3.7	41
16	General Computational Algorithms for Ab Initio Crystal Structure Prediction for Organic Molecules. Topics in Current Chemistry, 2014, 345, 25-58.	4.0	31
17	Optimal Site Charge Models for Molecular Electrostatic Potentials. Molecular Simulation, 2004, 30, 413-436.	0.9	29
18	Crystal Structure Prediction Methods for Organic Molecules: State of the Art. Annual Review of Chemical and Biomolecular Engineering, 2021, 12, 593-623.	3.3	28

#	Article	IF	Citations
19	Accurate and efficient representation of intramolecular energy inab initiogeneration of crystal structures. I. Adaptive local approximate models. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 864-874.	0.5	18
20	Efficient Screening of Coformers for Active Pharmaceutical Ingredient Cocrystallization. Crystal Growth and Design, 2022, 22, 4513-4527.	1.4	14
21	Optimisation-based scheduling: A discrete manufacturing case study. Computers and Industrial Engineering, 2005, 49, 118-145.	3.4	12
22	Dynamic modelling of aqueous electrolyte systems. Computers and Chemical Engineering, 2003, 27, 869-882.	2.0	9
23	Accurate and efficient representation of intramolecular energy in ab initio generation of crystal structures. II. Smoothed intramolecular potentials. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 423-433.	0.5	9
24	Repulsionâ€“dispersion parameters for the modelling of organic molecular crystals containing N, O, S and Cl. Faraday Discussions, 2018, 211, 297-323.	1.6	7
25	A tribute to professor Roger Sargent: Intellectual leader of process systems engineering. AICHE Journal, 2016, 62, 2951-2958.	1.8	6
26	Consistency on Domain Boundaries for Linear PDAE Systems. SIAM Journal of Scientific Computing, 2008, 30, 916-936.	1.3	3
27	Molecular Dynamics as a Mathematical Mapping. II. Partial Derivatives in the Microcanonical Ensemble. Molecular Simulation, 2001, 26, 167-192.	0.9	2
28	Efficient Parameterization of a Surrogate Model of Molecular Interactions in Crystals. Computer Aided Chemical Engineering, 2020, , 493-498.	0.3	2
29	Molecular Dynamics as a Mathematical Mapping. III. Efficient Evaluation of the Differentiable Force Functions and Their Derivatives. Molecular Simulation, 2001, 26, 323-352.	0.9	1
30	Molecular Dynamics as a Mathematical Mapping. I. Differentiable Force Functions. Molecular Simulation, 2001, 26, 237-271.	0.9	1
31	Consistency of general point conditions for DAE systems. Computers and Chemical Engineering, 2005, 30, 125-136.	2.0	1