Thuat T Trinh

List of Publications by Year
in descending order

61 papers	1,515 citations	279701 23 h-index	330025 37 g-index
63 all docs	63 docs citations	63 times ranked	1815 citing authors

#	Article	IF	Citations
1	Mechanism of Oligomerization Reactions of Silica. Journal of Physical Chemistry B, 2006, 110, 23099-23106.	1.2	140
2	Mechanism of the Initial Stage of Silicate Oligomerization. Journal of the American Chemical Society, 2011, 133, 6613-6625.	6.6	99
3	Effects of wet torrefaction on pyrolysis of woody biomass fuels. Energy, 2015, 88, 443-456.	4.5	93
4	Mechanical instability of monocrystalline and polycrystalline methane hydrates. Nature Communications, 2015, 6, 8743.	5.8	93
5	The role of water in silicate oligomerization reaction. Physical Chemistry Chemical Physics, 2009, 11, 5092.	1.3	72
6	Role of Water in Silica Oligomerization. Journal of Physical Chemistry C, 2009, 113, 2647-2652.	1.5	67
7	Non-isothermal pyrolysis of torrefied stump â€“ A comparative kinetic evaluation. Applied Energy, 2014, 136, 759-766.	5.1	65
8	Aromatic Gain in a Supramolecular Polymer. Angewandte Chemie - International Edition, 2015, 54, 10502-10506.	7.2	57
9	Effect of Counter Ions on the Silica Oligomerization Reaction. ChemPhysChem, 2009, 10, 1775-1782.	1.0	46
10	Structure-Directing Role of Counterions in the Initial Stage of Zeolite Synthesis. Journal of Physical Chemistry C, 2011, 115, 9561-9567.	1.5	42
11	The initial step of silicate versus aluminosilicate formation in zeolite synthesis: a reaction mechanism in water with a tetrapropylammonium template. Physical Chemistry Chemical Physics, 2012, 14, 3369.	1.3	40
12	Low barriers for hydrogen diffusion in sII clathrate. Physical Chemistry Chemical Physics, 2015, 17, 13808-13812.	1.3	34
13	Density Functional Theory Study on the Interactions of Metal Ions with Long Chain Deprotonated Carboxylic Acids. Journal of Physical Chemistry A, 2015, 119, 10195-10203.	1.1	33
14	Clarifying the role of sodium in the silica oligomerization reaction. Physical Chemistry Chemical Physics, 2013, 15, 1123-1129.	1.3	31
15	Influence of Curvature on the Transfer Coefficients for Evaporation and Condensation of Lennard-Jones Fluid from Square-Gradient Theory and Nonequilibrium Molecular Dynamics. Journal of Physical Chemistry C, 2015, 119, 8160-8173.	1.5	28
16	Ab Initio Molecular Dynamics Study on the Interactions between Carboxylate Ions and Metal Ions in Water. Journal of Physical Chemistry B, 2015, 119, 10710-10719.	1.2	28
17	The role of a structure directing agent tetramethylammonium template in the initial steps of silicate oligomerization in aqueous solution. Physical Chemistry Chemical Physics, 2015, 17, 21810-21818.	1.3	27
18	Rare event simulations reveal subtle key steps in aqueous silicate condensation. Physical Chemistry Chemical Physics, 2017, 19, 13361-13371.	1.3	27

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19	Thiosquaramide-Based Supramolecular Polymers: Aromaticity Gain in a Switched Mode of Self-Assembly. Journal of the American Chemical Society, 2020, 142, 19907-19916.	6.6	26
20	Heat transport through a solidâ€“solid junction: the interface as an autonomous thermodynamic system. Physical Chemistry Chemical Physics, 2016, 18, 13741-13745.	1.3	25
21	Selectivity and self-diffusion of CO2 and H2 in a mixture on a graphite surface. Frontiers in Chemistry, 2013, 1, 38.	1.8	24
22	The relative stability of zeolite precursor tetraalkylammoniumâ€“silicate oligomer complexes. Microporous and Mesoporous Materials, 2011, 146, 82-87.	2.2	23
23	Coherent description of transport across the water interface: From nanodroplets to climate models. Physical Review E, 2016, 93, 032801.	0.8	23
24	Thermal conductivity of carbon dioxide from non-equilibrium molecular dynamics: A systematic study of several common force fields. Journal of Chemical Physics, 2014, 141, 134504.	1.2	21
25	A test on reactive force fields for the study of silica dimerization reactions. Journal of Chemical Physics, 2015, 143, 184113.	1.2	19
26	Heat and Mass Transfer across Interfaces in Complex Nanogeometries. Physical Review Letters, 2015, 114, 065901.	2.9	19
27	Fuel characterization and thermal degradation kinetics of biomass from phytoremediation plants. Biomass and Bioenergy, 2020, 134, 105469.	2.9	19
28	Elastic and thermodynamic properties of the major clinker phases of Portland cement: Insights from first principles calculations. Construction and Building Materials, 2021, 287, 122873.	3.2	18
29	Diffusion of gas mixtures in the sI hydrate structure. Journal of Chemical Physics, 2018, 148, 214701.	1.2	17
30	Bridging scales with thermodynamics: from nano to macro. Advances in Natural Sciences: Nanoscience and Nanotechnology, 2014, 5, 023002.	0.7	15
31	Application of electrochemical oxidation in cold climate regions â€“ Effect of temperature, pH and anode material on the degradation of Bisphenol A and the formation of disinfection by-products. Journal of Environmental Chemical Engineering, 2020, 8, 104183.	3.3	15
32	Energy crops for sustainable phytoremediation â€“ Thermal decomposition kinetics. Energy Procedia, 2019, 158, 873-878.	1.8	14
33	Calculation of the chemical potential and the activity coefficient of two layers of CO₂ adsorbed on a graphite surface. Physical Chemistry Chemical Physics, 2015, 17, 1226-1233.	1.3	12
34	A Molecular Dynamics Simulation Study on Separation Selectivity of CO2/CH4 Mixture in Mesoporous Carbons. Energy Procedia, 2016, 86, 144-149.	1.8	12
35	Graphene coatings for chemotherapy: avoiding silver-mediated degradation. 2D Materials, 2015, 2, 025004.	2.0	11
36	Elucidating the Role of Tetraethylammonium in the Silicate Condensation Reaction from Ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2020, 124, 10210-10218.	1.2	11

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37	Insights into the Kinetics of Intermediate Formation during Electrochemical Oxidation of the Organic Model Pollutant Salicylic Acid in Chloride Electrolyte. Water (Switzerland), 2019, 11, 1322.	1.2	10
38	How do the doping concentrations of N and B in graphene modify the water adsorption?. RSC Advances, 2021, 11, 19560-19568.	1.7	10
39	Simulation of Pore Width and Pore Charge Effects on Selectivities of CO2 vs. H2 from a Syngas-like Mixture in Carbon Mesopores. Energy Procedia, 2015, 64, 150-159.	1.8	9
40	Correlation between the porosity of Î³-Al2O3 and the performance of CuOâ€“ZnOâ€“Al2O3 catalysts for CO2 hydrogenation into methanol. Reaction Kinetics, Mechanisms and Catalysis, 2018, 124, 171-185.	0.8	9
41	Impact of Organic Templates on the Selective Formation of Zeolite Oligomers. Angewandte Chemie, 2021, 133, 7187-7192.	1.6	9
42	Thermodynamic characterization of two layers of CO2 on a graphite surface. Chemical Physics Letters, 2014, 612, 214-218.	1.2	8
43	On the relation between the Langmuir and thermodynamic flux equations. Frontiers in Physics, 2014, 1, .	1.0	7
44	The mechanism of the initial step of germanosilicate formation in solution: a first-principles molecular dynamics study. Physical Chemistry Chemical Physics, 2016, 18, 14419-14425.	1.3	7
45	Impact of Organic Templates on the Selective Formation of Zeolite Oligomers. Angewandte Chemie - International Edition, 2021, 60, 7111-7116.	7.2	7
46	Mechanism of proton transport in water clusters and the effect of electric fields: A DFT study. Current Applied Physics, 2021, 25, 62-69.	1.1	7
47	Effect of hydrogen-bonding networks in water on the proton conductivity properties of metalâ€“organic frameworks. Journal of Science: Advanced Materials and Devices, 2021, 6, 509-515.	1.5	7
48	Reply to â€œComment on 'Structure-Directing Role of Counterions in the Initial Stage of Zeolite Synthesisâ€• Journal of Physical Chemistry C, 2012, 116, 1622-1623.	1.5	6
49	A procedure to find thermodynamic equilibrium constants for CO₂ and CH₄ adsorption on activated carbon. Physical Chemistry Chemical Physics, 2015, 17, 8223-8230.	1.3	6
50	Thermodynamic properties of hydrogen dissociation reaction from the small system method and reactive force field ReaxFF. Chemical Physics Letters, 2017, 672, 128-132.	1.2	6
51	Geometrical flexibility of platinum nanoclusters: impacts on catalytic decomposition of ethylene glycol. Physical Chemistry Chemical Physics, 2017, 19, 28596-28603.	1.3	6
52	Finite-size and truncation effects for microscopic expressions for the temperature at equilibrium and nonequilibrium. Journal of Chemical Physics, 2015, 143, 114106.	1.2	5
53	Chemically accurate energy barriers of small gas molecules moving through hexagonal water rings. Physical Chemistry Chemical Physics, 2016, 18, 17831-17835.	1.3	5
54	CFD pre-study of Nozzle reactor for fast hydrothermal liquefaction. Energy Procedia, 2017, 142, 861-866.	1.8	5

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55	Degradation of the chemotherapy drug 5-fluorouracil on medical-grade silver surfaces. Applied Surface Science, 2018, 435, 1213-1219.	3.1	5
56	Initial degradation mechanism of salicylic acid via electrochemical process. Chemical Physics, 2021, 543, 111071.	0.9	4
57	Temperature anisotropy at equilibrium reveals nonlocal entropic contributions to interfacial properties. Physical Review E, 2018, 97, 012126.	0.8	3
58	Note: A new truncation correction for the configurational temperature extends its applicability to interaction potentials with a discontinuous force. Journal of Chemical Physics, 2016, 144, 056101.	1.2	1
59	Selective dissolution of woody biomass under hydrothermal conditions. Energy Procedia, 2017, 142, 867-872.	1.8	1
60	Coverage degrees of colloids on electrochemical electrodes and signal amplification for anti-citrullinated peptide antibody detection. Sensing and Bio-Sensing Research, 2020, 27, 100322.	2.2	1
61	RÃ¼cktitelbild: Impact of Organic Templates on the Selective Formation of Zeolite Oligomers (Angew.) Tj ETQq1 1 0.784314 rgBT /O	1.6	0