Ole Swang

List of Publications by Year in descending order

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67 papers	2,471 citations	236925 25 h-index	206112 48 g-index
70 all docs	70 docs citations	70 times ranked	2991 citing authors

#	Article	IF	Citations
1	Unimolecular Decomposition Reactions of Picric Acid and Its Methylated Derivativesâ”€A DFT Study. Journal of Physical Chemistry A, 2022, 126, 2645-2657.	2.5	5
2	Structure, hydration, and chloride ingress in C-S-H: Insight from DFT calculations. Cement and Concrete Research, 2020, 129, 105965.	11.0	30
3	Surface Reconstruction, Hydration, and Adhesion of Epoxy to the (0001) Surface of Î±-Berlinite: Insights from Density Functional Theory Calculations. Journal of Physical Chemistry C, 2020, 124, 6683-6688.	3.1	1
4	Synthesis and characterization of Al@MOF materials. Materials Chemistry and Physics, 2019, 226, 220-225.	4.0	13
5	Desilication of SAPO-34: Reaction Mechanisms from Periodic DFT Calculations. Journal of Physical Chemistry C, 2015, 119, 2073-2085.	3.1	23
6	Mechanism of Si Island Formation in SAPO-34. Journal of Physical Chemistry C, 2015, 119, 2086-2095.	3.1	33
7	Kinetics of Zeolite Dealumination: Insights from H-SSZ-13. ACS Catalysis, 2015, 5, 7131-7139.	11.2	69
8	Correction to â€œMechanism of Si Island Formation in SAPO-34â€. Journal of Physical Chemistry C, 2015, 119, 20782-20782.	3.1	0
9	Oxygenâ€Promoted Cï£¿H Bond Activation at Palladium. Angewandte Chemie - International Edition, 2014, 53, 6492-6495.	13.8	26
10	Mechanistic Comparison of the Dealumination in SSZ-13 and the Desilication in SAPO-34. Journal of Physical Chemistry C, 2013, 117, 13442-13451.	3.1	62
11	Unit cell expansion upon coke formation in a SAPO-34 catalyst: A combined experimental and computational study. Microporous and Mesoporous Materials, 2013, 165, 1-5.	4.4	32
12	Rock â€˜nâ€™ Roll With Gold: Synthesis, Structure, and Dynamics of a (bipyridine)AuCl3 Complex. Organometallics, 2012, 31, 7093-7100.	2.3	18
13	Stabilization of Silicon Islands in Silicoaluminophosphates by Proton Redistribution. Journal of Physical Chemistry C, 2012, 116, 7255-7259.	3.1	19
14	A computational study on heteroatom distribution in zeotype materials. Microporous and Mesoporous Materials, 2012, 158, 175-179.	4.4	14
15	Detailed Reaction Paths for Zeolite Dealumination and Desilication From Density Functional Calculations. Angewandte Chemie - International Edition, 2012, 51, 652-655.	13.8	101
16	Chemisorption on cobalt surfaces: The effect of subsurface rhenium atoms from quantum chemical cluster model calculations. Surface Science, 2011, 605, 513-519.	1.9	3
17	Gold(iii) six-membered NâCâN pincer complexes: synthesis, structure, reactivity and theoretical calculations. Dalton Transactions, 2010, 39, 10293.	3.3	24
18	Bimetallic Cobalt/Rhenium Systems: Preferred Position of Rhenium Through an Interdisciplinary Approach. Catalysis Letters, 2010, 135, 21-25.	2.6	11

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19	Thermochemistry of Organic Reactions in Microporous Oxides by Atomistic Simulations: Benchmarking against Periodic B3LYP. Journal of Physical Chemistry A, 2010, 114, 7391-7397.	2.5	21
20	(Î²-Diketiminato)dimethylgold(III): Synthesis, Structure, and Reactivity. Organometallics, 2010, 29, 2248-2253.	2.3	19
21	Ping-Pong at Gold: Proton Jump Between Coordinated Phenyl and Î·¹-Benzene Ligands, A Computational Study. Journal of Physical Chemistry A, 2010, 114, 8135-8141.	2.5	11
22	Amine functionalised metal organic frameworks (MOFs) asÂadsorbents for carbon dioxide. Adsorption, 2008, 14, 755-762.	3.0	409
23	On the Nonsingle-Site Character of Bis(2-Dimethylsilyl-indenyl)zirconium(IV) Dichloride/MAO and Bis(2-Trimethylsilyl-indenyl)zirconium(IV) Dichloride/MAO:â€‰ Polymerization Characteristics and Mechanistic Implications. Journal of Physical Chemistry A, 2008, 112, 4074-4089.	2.5	5
24	Atomistic and electronic structure of bimetallic cobalt/rhenium clusters from density functional theory calculations. Journal of Chemical Physics, 2008, 128, 084712.	3.0	10
25	CO2Absorption in Aqueous Solutions of Alkanolamines:Â Mechanistic Insight from Quantum Chemical Calculations. Journal of Physical Chemistry A, 2007, 111, 1222-1228.	2.5	173
26	A general one-pot synthesis for elusive 2-substituted indenes: does bis[2-(tert-butyl)indenyl]zirconium(iv) dichloride/MAO polymerise ethene?. Dalton Transactions, 2006, , 2098-2105.	3.3	8
27	An Experimental and Theoretical Study of Spinâ^'Spin Coupling in Chlorosilanes. Journal of Physical Chemistry A, 2006, 110, 9801-9804.	2.5	10
28	Theoretical study of carbon atom scrambling in benzenium ions with ethyl or isopropyl groups. Journal of Physical Organic Chemistry, 2006, 19, 81-92.	1.9	11
29	Oxygen influence on the dissociative chemisorption of methane on nickel: A quantum chemical cluster model study. Chemical Physics Letters, 2006, 432, 94-99.	2.6	3
30	Synthetic Explorations Towards Sterically Crowded 1,2,3-Substituted Bis(indenyl)zirconium(IV) Dichlorides. European Journal of Inorganic Chemistry, 2005, 2005, 1759-1769.	2.0	10
31	Methylation of Alkenes and Methylbenzenes by Dimethyl Ether or Methanol on Acidic Zeolites. Journal of Physical Chemistry B, 2005, 109, 12874-12878.	2.6	98
32	Theoretical Study of the Heptamethylbenzenium Ion. Intramolecular Isomerizations and C2, C3, C4Alkene Elimination. Journal of Physical Chemistry A, 2005, 109, 8914-8922.	2.5	41
33	Modeling alkali alanates for hydrogen storage by density-functional band-structure calculations. Journal of Materials Research, 2005, 20, 3199-3213.	2.6	41
34	CO2 Sorption on MgO and CaO Surfaces:â€‰ A Comparative Quantum Chemical Cluster Study. Journal of Physical Chemistry B, 2005, 109, 16774-16781.	2.6	142
35	Theoretical study of protonated xylenes: ethene elimination and H,Câ€scrambling reactions. Journal of Physical Organic Chemistry, 2004, 17, 1023-1032.	1.9	29
36	Synthesis, structure, and ethene polymerisation catalysis of 1- or 2-silyl substituted bis[indenyl]zirconium(iv) dichlorides. Dalton Transactions, 2004, , 1578-1589.	3.3	11

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37	Theoretical Investigation of Arene Alkylation by Ethene and Propene over Acidic Zeolites. Journal of Physical Chemistry B, 2004, 108, 2300-2308.	2.6	33
38	Theoretical Investigation of the Dimerization of Linear Alkenes Catalyzed by Acidic Zeolites. Journal of Physical Chemistry B, 2004, 108, 2953-2962.	2.6	78
39	The performance of density functional theory for LnF (Ln=Nd, Eu, Gd, Yb) and YbH. Theoretical Chemistry Accounts, 2003, 110, 118-125.	1.4	41
40	Molecular Structures of Two Metal Tetrakis(tetrahydroborates), Zr(BH4)4 and U(BH4)4: Equilibrium Conformations and Barriers to Internal Rotation of the Triply Bridging BH4 Groups. ChemInform, 2003, 34, no.	0.0	0
41	Heterolytic activation of C?H bond in methane with (HN?CHCH?NH)M(CH3) (M = Pd+, Pt+, Rh+, Ir+, Rh,) Tj ETQq1 1 0.784314 rgBT /O Chemistry, 2003, 92, 391-399.	2.0	15
42	A Theoretical Investigation of the Methylation of Alkenes with Methanol over Acidic Zeolites. Journal of Physical Chemistry B, 2003, 107, 9281-9289.	2.6	71
43	A Theoretical Investigation of the Methylation of Methylbenzenes and Alkenes by Halomethanes over Acidic Zeolites. Journal of Physical Chemistry B, 2003, 107, 5251-5260.	2.6	61
44	A Theoretical Investigation on the Methylation of Methylbenzenes on Zeolites. Journal of Physical Chemistry B, 2002, 106, 12722-12726.	2.6	52
45	Molecular Structures of Two Metal Tetrakis(tetrahydroborates), Zr(BH4)4and U(BH4)4:Â Equilibrium Conformations and Barriers to Internal Rotation of the Triply Bridging BH4Groups. Inorganic Chemistry, 2002, 41, 6646-6655.	4.0	43
46	Semi-Batch Polymerisations of Ethylene with Metallocene Catalysts in the Presence of Hydrogen, 3. Correlation Between Hydrogen Sensitivity and Molecular Parameters. Macromolecular Chemistry and Physics, 2002, 203, 381-387.	2.2	11
47	Dynamic Behaviour of Tris(2-methylallyl)chromium â^' NMR and DFT Results. European Journal of Inorganic Chemistry, 2002, 2002, 411-415.	2.0	7
48	On the Gas-Phase Chlorination of Ethane. Industrial & Engineering Chemistry Research, 2001, 40, 2226-2235.	3.7	19
49	Methyl Side Chain Formation on the CrCp2/SiO2 Catalyst during Polymerisation of Ethylene: Spectroscopic Analyses and Theoretical Modelling. Journal of Catalysis, 2000, 194, 352-363.	6.2	9
50	A Combined Experimental and Density Functional Theory Investigation of Hydrocarbon Activation at a Cationic Platinum(II) Diimine Aqua Complex under Mild Conditions in a Hydroxylic Solvent. Journal of the American Chemical Society, 2000, 122, 10831-10845.	13.7	120
51	Câ^'H Activation at a Cationic Platinum (II) Center:Â A Quantum Chemical Investigation. Journal of Physical Chemistry A, 1999, 103, 10004-10008.	2.5	29
52	Allyl complexes of chromium and zirconium: molecular structures from DFT and ab initio calculations. Journal of Organometallic Chemistry, 1998, 561, 29-35.	1.8	10
53	Substituent crowding in nitrobenzenes. Journal of Molecular Structure, 1998, 445, 89-98.	3.6	12
54	A computational study of the molecular structures, conformational preferences and anomeric effects in mono- and bisaminophosphanes. Journal of Molecular Structure, 1998, 445, 303-309.	3.6	16

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55	The molecular structures of tris(dimethylamino)-phosphane, -arsane and -stibane, E(NMe2)3, E î—» P, As or Sb and Me î—» CH3, by gas electron diffraction and ab initio molecular orbital calculations. Journal of Molecular Structure, 1998, 445, 311-317.	3.6	18
56	On the Nature and Incidence of Î²-Agostic Interactions in Ethyl Derivatives of Early Transition Metals:Â Ethyltitanium Trichloride and Related Compounds. Journal of the American Chemical Society, 1998, 120, 3762-3772.	13.7	84
57	Molecular structures of the sixth period metal pentachlorides, MCl5 (Mâ€…=â€…Ta, W or Re), determined by gas electron diffraction; is Jahnâ€“Teller distortion of WCl5 quenched by spinâ€“orbit coupling?. Journal of the Chemical Society Dalton Transactions, 1997, , 1013-1018.	1.1	18
58	Molecular Structure and Câ‹¯O Stretch Frequencies of the Cobalt Carbonyls Co(CO)n, n = 1, 4, As Studied by Density Functional Theory. Journal of Physical Chemistry A, 1997, 101, 8956-8958.	2.5	18
59	Evaluation of PM3(tm) as a Geometry Generator in Theoretical Studies of Transition-Metal-Based Catalysts for Polymerizing Olefins. Journal of Molecular Modeling, 1997, 3, 193-202.	1.8	25
60	Solvation of Palladium Diacetate in Trifluoroacetic Acid. The Journal of Physical Chemistry, 1996, 100, 17334-17336.	2.9	20
61	Chemisorption of hydrogen and oxygen atoms on a cobalt surface: A quantum chemical cluster model study. International Journal of Quantum Chemistry, 1996, 57, 105-111.	2.0	9
62	RECP calculations for reactions of H2 with Pt, Os, Ir, and Re ? a systematic comparison. Theoretica Chimica Acta, 1995, 91, 109-110.	0.8	0
63	Molecular structure of monomeric uranium tetrachloride determined by gas electron diffraction at 900 K, gasphase infrared spectroscopy and quantum-chemical density-functional calculations. Journal of the Chemical Society Dalton Transactions, 1995, , 185.	1.1	21
64	Theoretical Study of Methane Activation by Re, Os, Ir, and Pt. The Journal of Physical Chemistry, 1994, 98, 3006-3009.	2.9	11
65	Theoretical cluster model studies of bimetallic heterogeneous catalysis: dissociation of hydrogen on a rhenium-doped nickel cluster. Chemical Physics Letters, 1993, 207, 397-402.	2.6	1
66	Molecular Structure of Pentamethylantimony by Gas Electron Diffraction; Structure and Bonding in Sb(CH3)5 and Bi(CH3)5 Studied by Ab Initio MO Calculations.. Acta Chemica Scandinavica, 1993, 47, 368-373.	0.7	15
67	A theoretical study of the chemisorption of methane on a Ni(100) surface. Chemical Physics, 1991, 156, 379-386.	1.9	49