Mats Svensson

List of Publications by Year in descending order

38 papers	4,248 citations	236612 25 h-index	329751 37 g-index
39 all docs	39 docs citations	39 times ranked	3840 citing authors

#	Article	IF	Citations
1	ONIOM:Â A Multilayered Integrated MO + MM Method for Geometry Optimizations and Single Point Energy Predictions. A Test for Dielsâ^'Alder Reactions and Pt(P(t-Bu)3)2+ H2Oxidative Addition. The Journal of Physical Chemistry, 1996, 100, 19357-19363.	2.9	1,824
2	Energetics using the single point IMOMO (integrated molecular orbital+molecular orbital) calculations: Choices of computational levels and model system. Journal of Chemical Physics, 1996, 105, 3654-3661.	1.2	282
3	A Density Functional Study of the Mechanism of the Diimineâ^'Nickel-Catalyzed Ethylene Polymerization Reaction. Journal of the American Chemical Society, 1997, 119, 367-374.	6.6	181
4	Mechanism of Ring-Opening Polymerization of 1,5-Dioxepan-2-one and l-Lactide with Stannous 2-Ethylhexanoate. A Theoretical Study. Macromolecules, 2001, 34, 3877-3881.	2.2	164
5	Mechanisms for the reactions between methane and the neutral transition metal atoms from yttrium to palladium. Journal of the American Chemical Society, 1992, 114, 6095-6102.	6.6	145
6	PCI-X, a parametrized correlation method containing a single adjustable parameter X. Chemical Physics Letters, 1994, 223, 35-45.	1.2	115
7	IMOMO(G2MS):â€‰ A New High-Level G2-Like Method for Large Molecules and Its Applications to Dielsâ^'Alder Reactions. Journal of Physical Chemistry A, 1997, 101, 227-233.	1.1	112
8	Density Functional Study of the Mechanism of the Palladium(II)-Catalyzed Ethylene Polymerization Reaction. Organometallics, 1997, 16, 1933-1945.	1.1	109
9	Comparisons of results from parametrized configuration interaction (PCIâ€80) and from hybrid density functional theory with experiments for first row transition metal compounds. Journal of Chemical Physics, 1996, 104, 9546-9554.	1.2	103
10	Nitrogen Fixation by Nitrogenases:â€‰ A Quantum Chemical Study. Journal of Physical Chemistry B, 1998, 102, 1615-1623.	1.2	97
11	Ring-Opening Polymerization of Lactones and Lactides with Sn(IV) and Al(III) Initiators. Macromolecules, 2002, 35, 1556-1562.	2.2	88
12	An Exploratory Study of Regiocontrol in the Heck Type Reaction. Influence of Solvent Polarity and Bisphosphine Ligands. Organometallics, 1999, 18, 970-975.	1.1	87
13	A theoretical study of the activation of the carbon-hydrogen bond in ethylene by second-row transition-metal atoms. Journal of the American Chemical Society, 1993, 115, 1952-1958.	6.6	85
14	Electronic Control of the Regiochemistry in the Heck Reaction. Journal of the American Chemical Society, 2003, 125, 3503-3508.	6.6	83
15	The effects of covalent ligands on the oxidative addition reaction between second-row transition-metal atoms and methane. Journal of the American Chemical Society, 1993, 115, 4191-4200.	6.6	81
16	Insertion Aptitudes and Insertion Regiochemistry of Various Alkenes Coordinated to Cationic (Ïƒ-R)(diimine)palladium(II) (R = â^'CH3, â^'C6H5). A Theoretical Study. Organometallics, 2001, 20, 2813-2819.	1.1	81
17	Theoretical Study of Pd(II)- and Ni(II)-Catalyzed Alternating Copolymerization of Carbon Monoxide with Ethylene. Organometallics, 1996, 15, 5568-5576.	1.1	76
18	First row benchmark tests of the parametrized configuration interaction with parameter X (PCIâ€X) scheme. Journal of Chemical Physics, 1995, 102, 5377-5386.	1.2	66

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19	Experimental and theoretical study of oxidative addition reaction of nickel atom to Oâ€“H bond of water. Journal of Chemical Physics, 1994, 100, 423-433.	1.2	49
20	Electronic and Steric Ligand Effects on the Activity and Regiochemistry in the Heck Reaction. Organometallics, 2002, 21, 2248-2253.	1.1	43
21	Binding of Ethylene to Anionic, Neutral, and Cationic Nickel(II), Palladium(II), and Platinum(II)cis/transChloride Ammonia Complexes. A Theoretical Study. Organometallics, 1997, 16, 3165-3168.	1.1	42
22	Validation of a Computational Model for Predicting the Site for Electrophilic Substitution in Aromatic Systems. Journal of Organic Chemistry, 2010, 75, 4696-4705.	1.7	42
23	Geometry optimization for second-row transition metal complexes. Chemical Physics Letters, 1993, 216, 147-154.	1.2	37
24	Predicting Regioselectivity in Nucleophilic Aromatic Substitution. Journal of Organic Chemistry, 2012, 77, 3262-3269.	1.7	37
25	Analytical Second Derivatives for Effective Core Potential. Application to Transition Structures of Cp2Ru2(Î¼-H)4and to the Mechanism of Reaction Cu + CH2N2. The Journal of Physical Chemistry, 1996, 100, 10936-10944.	2.9	35
26	The interaction of ammonia, carbonyl, ethylene and water with the copper and silver dimers. Chemical Physics Letters, 1994, 231, 337-344.	1.2	25
27	(Hydroxyalkyl)pyridinooxazolines in Palladium-Catalyzed Allylic Substitutions. Conformational Preferences of the Ligand. Organometallics, 1999, 18, 4900-4907.	1.1	22
28	Asymmetric Catalysis Special Feature Part I: OH-Pd(0) interaction as a stabilizing factor in palladium-catalyzed allylic alkylations. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 5400-5404.	3.3	22
29	Potency Prediction of Î²-Secretase (BACE-1) Inhibitors Using Density Functional Methods. Journal of Chemical Information and Modeling, 2014, 54, 818-825.	2.5	20
30	Utilizing the Ïƒ-complex stability for quantifying reactivity in nucleophilic substitution of aromatic fluorides. Beilstein Journal of Organic Chemistry, 2013, 9, 791-799.	1.3	19
31	A pragmatic procedure for predicting regioselectivity in nucleophilic substitution of aromatic fluorides. Tetrahedron Letters, 2011, 52, 3150-3153.	0.7	18
32	A Proton Directly Attacks 1,5-Cyclooctadiene in Bis(1,5-cyclooctadiene)nickel(0) in the Formation of a Keim Type Oligomerization Catalyst. Organometallics, 1998, 17, 5367-5373.	1.1	16
33	On the internally contracted multireferenceCI method with full contraction. International Journal of Quantum Chemistry, 1992, 41, 153-162.	1.0	15
34	Creation of Novel Cores for Î²-Secretase (BACE-1) Inhibitors: A Multiparameter Lead Generation Strategy. ACS Medicinal Chemistry Letters, 2014, 5, 440-445.	1.3	12
35	Synthesis of 2,3-Dihydrothieno[2,3-b]-1,4-dithiine, 2,3-Dihydrothieno-[3,2-b]-1,4-oxathiine, 2,3-Dihydrothieno[2,3-b]-1,4-oxathiine and Their TransformationÂ-into Corresponding End-Capped Oligomers. Synthesis, 2003, 2003, 2199-2205.	1.2	10
36	A simple and versatile protocol for the preparation of 1,3-functionalized heterocycles utilizing benzoylpyruvates. Journal of Heterocyclic Chemistry, 2010, 47, 878-886.	1.4	3

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37	Theoretical Studies of the N2 Cleavage by Three-Coordinate Group 6 Complexes ML3. ACS Symposium Series, 1999, , 198-207.	0.5	2
38	Synthesis of 2,3-Dihydrothieno[2,3-b]-1,4-dithiine, 2,3-Dihydrothieno[3,2-b]-1,4-oxathiine, 2,3-Dihydrothieno[2,3-b]-1,4-oxathiine and Their Transformation into Corresponding End-Capped Oligomers.. ChemInform, 2004, 35, no.	0.1	0