Citation Report

Grajciar L* (Author)

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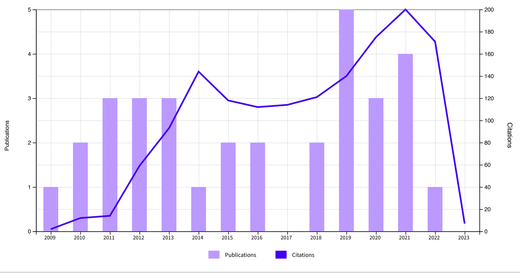

32 Publications

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1 of 1

		Citations						
		Previous year				Next year	Average per year	Total
		2019	2020	2021	2022	2023		
	Total	140	175	200	171	7	98.8	1,482
1	Accurate large-scale simulations of siliceous zeolites by neural network potentials Erlebach, A; Nachtigall, P and Grajciar, L Aug 19 2022 | NPJ COMPUTATIONAL MATERIALS 8 (1)	0	0	0	1	0	0.5	1
2	Mechanism of Zeolite Hydrolysis under Basic Conditions Jin, MT; Liu, MX; (...); Heard, CJ Dec 14 2021 | CHEMISTRY OF MATERIALS 33 (23) , pp.9202-9212	0	0	0	2	0	0.67	2
3	The Role of Water Loading and Germanium Content in Germanosilicate Hydrolysis Jin, MT; Vesely, O; (...); Grajciar, L Nov 4 2021 | Oct 2021 (Early Access) | JOURNAL OF PHYSICAL CHEMISTRY C 125 (43) , pp.23744-23757	0	0	1	2	0	1	3
4	Intrinsic valley polarization in 2D magnetic MXenes: surface engineering induced spin-valley coupling Li, S; He, JJ; (...); Nachtigall, P Sep 14 2021 | Jul 2021 (Early Access) | JOURNAL OF MATERIALS CHEMISTRY C 9 (34) , pp.11132-11141	0	0	1	10	1	4	12
5	Doping Isolated one-dimensional antiferromagnetic semiconductor vanadium tetrasulfide (VS4) nanowires with carriers induces half-metallicity Li, S; He, JJ; (...); Brivio, F Mar 7 2021 | JOURNAL OF MATERIALS CHEMISTRY C 9 (9) , pp.3122-3128	0	0	2	1	0	1	3
6	Origin of the Unusual Stability of Zeolite-Encapsulated Sub-Nanometer Platinum Hou, DW; Grajciar, L; (...); Heard, CJ Oct 2 2020 | ACS CATALYSIS 10 (19) , pp.11057-11068	0	1	3	7	0	2.75	11
7	Zeolite (In)Stability under Aqueous or Steaming Conditions Heard, CJ; Grajciar, L; (...); Nachtigall, P Nov 5 2020 | Aug 2020 (Early Access) | ADVANCED MATERIALS 32 (44)	0	0	15	8	1	6	24
8	Identification of the most active sites for tetrahydropyranylation in zeolites: MFI as a test case Liu, M; Vesely, O; (...); Grajciar, L 8th Czech-Italian-Spanish Symposium on Zeolites and Catalysis Apr 1 2020 | CATALYSIS TODAY 345 , pp.165-174	0	1	0	1	0	0.5	2
9	Control of spintronic and electronic properties of bimetallic and vacancy-ordered vanadium carbide MXenes via surface functionalization Li, S; He, JJ; (...); Brivio, F Dec 24 2019 | PHYSICAL CHEMISTRY CHEMICAL PHYSICS 21 (46) , pp.25802-25808	0	6	8	2	0	3.2	16
10	Structure Determination of the Oxygen Evolution Catalyst Mossbauerite Lou, PB; Eric, M; (...); Nachtigall, P Oct 17 2019 | JOURNAL OF PHYSICAL CHEMISTRY C 123 (41) , pp.25157-25165	0	2	3	0	0	1	5
11	Fast room temperature lability of aluminosilicate zeolites Heard, CJ; Grajciar, L; (...); Morris, RE Oct 16 2019 | NATURE COMMUNICATIONS 10	0	14	16	13	0	8.6	43
12	The Bronsted acidity of three- and two-dimensional zeolites Thang, HV; Vaculik, J; (...); Grajciar, L Jul 1 2019 | MICROPOROUS AND MESOPOROUS MATERIALS 282 , pp.121-132	0	7	3	5	0	3	15
13	The effect of water on the validity of Lowenstein's rule Heard, CJ; Grajciar, L and Nachtigall, P Jun 14 2019 | CHEMICAL SCIENCE 10 (22) , pp.5705-5711	3	5	13	6	0	5.4	27
14	Towards operando computational modeling in heterogeneous catalysis Grajciar, L; Heard, CJ; (...); Nachtigall, P Nov 21 2018 | CHEMICAL SOCIETY REVIEWS 47 (22) , pp.8307-8348	24	29	41	27	0	20.17	121
15	The Lewis acidity of three- and two-dimensional zeolites: The effect of framework topology Ho, TV; Nachtigall, P and Grajciar, L 7th Czech-Italian-Spanish Symposium on Zeolites and Catalysis Apr 15 2018 | CATALYSIS TODAY 304 , pp.12-21	2	4	2	1	0	1.83	11
16	PbS Clusters Embedded in Sodalite Zeolite Cavities of Different Compositions: Unraveling the Structural Evolution and Optical Properties Using ab Initio Calculations Grajciar, L Dec 1 2016 | JOURNAL OF PHYSICAL CHEMISTRY C 120 (47) , pp.27050-27065	2	2	1	3	0	1.5	12
17	Density Functional Theory for Molecular and Periodic Systems Using Density Fitting and Continuous Fast Multipole Method: Analytical Gradients Lazarski, R; Burow, AM; (...); Sierka, M Oct 30 2016 | JOURNAL OF COMPUTATIONAL CHEMISTRY 37 (28) , pp.2518-2526	4	4	4	2	0	2.25	18
18	Low-memory iterative density fitting Grajciar, L Jul 30 2015 | JOURNAL OF COMPUTATIONAL CHEMISTRY 36 (20) , pp.1521-1535	2	5	0	1	0	1.33	12
19	Accurate Ab Initio Description of Adsorption on Coordinatively Unsaturated Cu2+ and Fe3+ Sites in MOFs Grajciar, L; Nachtigall, P; (...); Rubes, M Jan 2015 | JOURNAL OF CHEMICAL THEORY AND COMPUTATION 11 (1) , pp.230-238	2	5	3	3	0	3.44	31
20	Adsorption of CO2 in FAU zeolites: Effect of zeolite composition Thang, HV; Grajciar, L; (...); Bulanek, R 5th Czech-Italian-Spanish-ICIS-IS Conference on Molecular Sieves and Catalysis (CIS-5) May 15 2014 | CATALYSIS TODAY 227 , pp.50-56	10	6	11	10	2	6.9	69
21	A family of zeolites with controlled pore size prepared using a top-down method Roth, WJ; Nachtigall, P; (...); Cejka, J Jul 2013 | NATURE CHEMISTRY 5 (7) , pp.628-633	30	34	24	23	0	27.18	299
22	Adsorption of Propane and Propylene on CuBTC Metal-Organic Framework: Combined Theoretical and Experimental Investigation Rubes, M; Wiersum, AD; (...); Nachtigall, P May 30 2013 | JOURNAL OF PHYSICAL CHEMISTRY C 117 (21) , pp.11159-11167	4	5	3	2	0	3.36	37
23	Theoretical investigation of layered zeolite frameworks: Interaction between IPC-1P layers derived from zeolite UTL Grajciar, L; Bludsky, O; (...); Nachtigall, P Apr 15 2013 | CATALYSIS TODAY 204 , pp.15-21	3	1	0	2	0	2.82	31
24	Combined Theoretical and Experimental Investigation of CO Adsorption on Coordinatively Unsaturated Sites in CuBTC MOF Rubes, M; Grajciar, L; (...); Nachtigall, P Feb 2012 | CHEMPHYSCHEM 13 (2) , pp.488-495	1	2	1	4	0	3.08	37
25	Controlling the Adsorption Enthalpy of CO2 in Zeolites by Framework Topology and Composition Grajciar, L; Cejka, J; (...); Nachtigall, P 2012 | CHEMSUSCHEM 5 (10) , pp.2011-2022	5	6	7	5	1	7.25	87
26	Control of CO2 adsorption heats by the Al distribution in FER zeolites: effect of synthesis conditions Nachtigall, P; Grajciar, L; (...); Cejka, J 2012 | PHYSICAL CHEMISTRY CHEMICAL PHYSICS 14 (3) , pp.1117-1120	3	0	2	1	0	2.08	25
27	Accurate Prediction of Methane Adsorption in a Metal-Organic Framework with Unsaturated Metal Sites by Direct Implementation of an ab Initio Derived Potential Energy Surface in GCMC Simulation Chen, L; Grajciar, L; (...); Duren, T Nov 24 2011 | JOURNAL OF PHYSICAL CHEMISTRY C 115 (46) , pp.23074-23080	5	2	1	2	0	5.92	77
28	Accurate Description of Argon and Water Adsorption on Surfaces of Graphene-Based Carbon Allotropes Kysilka, J; Rubes, M; (...); Bludsky, O Oct 20 2011 | JOURNAL OF PHYSICAL CHEMISTRY A 115 (41) , pp.11387-11393	7	3	7	2	1	4.85	63
29	Understanding CO2 Adsorption in CuBTC MOF: Comparing Combined DFT-ab Initio Calculations with Microcalorimetry Experiments Grajciar, L; Wiersum, AD; (...); Nachtigall, P Sep 15 2011 | JOURNAL OF PHYSICAL CHEMISTRY C 115 (36) , pp.17925-17933	9	13	10	6	1	9.77	127
30	Water Adsorption on Coordinatively Unsaturated Sites in CuBTC MOF Grajciar, L; Bludsky, O and Nachtigall, P Dec 2 2010 | JOURNAL OF PHYSICAL CHEMISTRY LETTERS 1 (23) , pp.3354-3359	9	11	8	11	0	10.43	146
31	Periodic DFT investigation of the effect of aluminium content on the properties of the acid zeolite H-FER Grajciar, L; Arean, CO; (...); Nachtigall, P 2010 | PHYSICAL CHEMISTRY CHEMICAL PHYSICS 12 (7) , pp.1497-1506	7	5	5	5	0	3.29	46
32	Computational and FTIR spectroscopic studies on carbon monoxide and dinitrogen adsorption on a high-silica H-FER zeolite Nachtigall, P; Bludsky, O; (...); Arean, CO 2009 | PHYSICAL CHEMISTRY CHEMICAL PHYSICS 11 (5) , pp.791-802	8	2	5	3	0	4.6	69

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