

Gert Jan Kramer

List of Publications by Year in descending order

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49
papers

6,530
citations

126907

33
h-index

214800

47
g-index

49
all docs

49
docs citations

49
times ranked

6326
citing authors

#	ARTICLE	IF	CITATIONS
1	Force fields for silicas and aluminophosphates based on ab initio calculations. <i>Physical Review Letters</i> , 1990, 64, 1955-1958.	7.8	1,366
2	Reactivity Theory of Zeolitic Brønsted Acidic Sites. <i>Chemical Reviews</i> , 1995, 95, 637-660.	47.7	575
3	The renaissance of the Sabatier reaction and its applications on Earth and in space. <i>Nature Catalysis</i> , 2019, 2, 188-197.	34.4	369
4	Zeolite Structure and Reactivity by Combined Quantum-Chemical and Classical Calculations. <i>Journal of Physical Chemistry B</i> , 1999, 103, 6133-6141.	2.6	343
5	Understanding the acid behaviour of zeolites from theory and experiment. <i>Nature</i> , 1993, 363, 529-531.	27.8	302
6	Cryogenic CO_2 capture using dynamically operated packed beds. <i>Chemical Engineering Science</i> , 2010, 65, 114-119.	3.8	242
7	Interatomic force fields for silicas, aluminophosphates, and zeolites: Derivation based on ab initio calculations. <i>Physical Review B</i> , 1991, 43, 5068-5080.	3.2	238
8	Life Cycle Inventory of the Production of Rare Earths and the Subsequent Production of NdFeB Rare Earth Permanent Magnets. <i>Environmental Science & Technology</i> , 2014, 48, 3951-3958.	10.0	209
9	No quick switch to low-carbon energy. <i>Nature</i> , 2009, 462, 568-569.	27.8	196
10	A multi-level perspective on the introduction of hydrogen and battery-electric vehicles. <i>Technological Forecasting and Social Change</i> , 2010, 77, 529-540.	11.6	184
11	Zeolites versus aluminosilicate clusters: the validity of a local description. <i>Journal of the American Chemical Society</i> , 1991, 113, 6435-6441.	13.7	181
12	Mechanisms of Hydrocarbon Conversion in Zeolites: A Quantum Mechanical Study. <i>Journal of Catalysis</i> , 1997, 170, 1-10.	6.2	181
13	Metal requirements of low-carbon power generation. <i>Energy</i> , 2011, 36, 5640-5648.	8.8	181
14	A critical view on the current application of LCA for new technologies and recommendations for improved practice. <i>Journal of Cleaner Production</i> , 2020, 259, 120904.	9.3	151
15	Theoretical determination of proton affinity differences in zeolites. <i>Journal of the American Chemical Society</i> , 1993, 115, 2887-2897.	13.7	146
16	Seasonal energy storage for zero-emissions multi-energy systems via underground hydrogen storage. <i>Renewable and Sustainable Energy Reviews</i> , 2020, 121, 109629.	16.4	137
17	Fischer-Tropsch technology from active site to commercial process. <i>Applied Catalysis A: General</i> , 1999, 186, 27-40.	4.3	129
18	Energy and Climate Impacts of Producing Synthetic Hydrocarbon Fuels from CO_2 . <i>Environmental Science & Technology</i> , 2014, 48, 7111-7121.	10.0	126

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19	Mechanisms for Chain Growth in Fischer–Tropsch Synthesis over Ru(0001). <i>Journal of Catalysis</i> , 2002, 212, 136-144.	6.2	119
20	Recycling Potential of Neodymium: The Case of Computer Hard Disk Drives. <i>Environmental Science & Technology</i> , 2014, 48, 9506-9513.	10.0	117
21	Framework for Resilience in Material Supply Chains, With a Case Study from the 2010 Rare Earth Crisis. <i>Environmental Science & Technology</i> , 2015, 49, 6740-6750.	10.0	117
22	An ab Initio Study of D/H Exchange between CD4 and the H-Forms of Zeolites FAU and MFI. <i>Journal of the American Chemical Society</i> , 1995, 117, 1766-1776.	13.7	113
23	Potential and challenges of low-carbon energy options: Comparative assessment of alternative fuels for the transport sector. <i>Applied Energy</i> , 2019, 236, 590-606.	10.1	92
24	Energetics of methane dissociative adsorption on Rh{111} from DFT calculations. <i>Journal of Catalysis</i> , 2006, 242, 309-318.	6.2	90
25	The influence of electronic structure on hydrogen absorption in palladium alloys. <i>Journal of Physics Condensed Matter</i> , 2004, 16, 6267-6277.	1.8	75
26	Evaluation of a Direct Air Capture Process Combining Wet Scrubbing and Bipolar Membrane Electrodialysis. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 7007-7020.	3.7	67
27	Absorption and diffusion of hydrogen in palladium-silver alloys by density functional theory. <i>Physical Review B</i> , 2002, 66, .	3.2	57
28	Novel Indicators for the Quantification of Resilience in Critical Material Supply Chains, with a 2010 Rare Earth Crisis Case Study. <i>Environmental Science & Technology</i> , 2017, 51, 3860-3870.	10.0	57
29	A Life Cycle Assessment Case Study of Coal-Fired Electricity Generation with Humidity Swing Direct Air Capture of CO ₂ versus MEA-Based Postcombustion Capture. <i>Environmental Science & Technology</i> , 2017, 51, 1024-1034.	10.0	49
30	Predictions of melting, crystallization, and local atomic arrangements of aluminum clusters using a reactive force field. <i>Journal of Chemical Physics</i> , 2008, 129, 244506.	3.0	47
31	Optimal hydrogen production in a wind-dominated zero-emission energy system. <i>Advances in Applied Energy</i> , 2021, 3, 100032.	13.2	36
32	Parametrization of a reactive force field for aluminum hydride. <i>Journal of Chemical Physics</i> , 2009, 131, 044501.	3.0	35
33	Two-section reactor model for autothermal reforming of methane to synthesis gas. <i>AIChE Journal</i> , 2003, 49, 1827-1837.	3.6	34
34	Why fully liberalised electricity markets will fail to meet deep decarbonisation targets even with strong carbon pricing. <i>Energy Policy</i> , 2019, 131, 99-110.	8.8	32
35	Modeling the sorption dynamics of NaH using a reactive force field. <i>Journal of Chemical Physics</i> , 2008, 128, 164714.	3.0	29
36	Comment on ‘‘How green is blue hydrogen?’’ <i>Energy Science and Engineering</i> , 2022, 10, 1944-1954.	4.0	23

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37	Energy scenariosâ€”Exploring disruption and innovation. Energy Research and Social Science, 2018, 37, 247-250.	6.4	15
38	Surface segregation in Pt ₂₅ Rh ₇₅ alloys studied by Monte Carlo simulations and the modified embedded atom method. Surface Science, 2007, 601, 1668-1676.	1.9	13
39	Construction of modified embedded atom method potentials for Cu, Pt and Cuâ€”Pt and modelling surface segregation in Cu ₃ Pt alloys. Surface Science, 2007, 601, 2952-2961.	1.9	13
40	An ab initio study of possible pathways in the thermal decomposition of NaAlH ₄ . Journal of Solid State Chemistry, 2008, 181, 3037-3043.	2.9	10
41	The climate resilience cycle: Using scenario analysis to inform climateâ€”resilient business strategies. Business Strategy and the Environment, 2022, 31, 1763-1775.	14.3	9
42	Shortcut model for water-balanced operation in fuel processor fuel cell systems. Journal of Power Sources, 2004, 138, 156-161.	7.8	7
43	Suppression of the Peierls Transition in MEM(TCNQ) ₂ Through Doping With METM. Molecular Crystals and Liquid Crystals, 1985, 120, 173-177.	0.8	5
44	Multiscale modeling of interaction of alane clusters on Al(111) surfaces: A reactive force field and infrared absorption spectroscopy approach. Journal of Chemical Physics, 2010, 132, 084509.	3.0	5
45	The 1-D Hubbard Model With Alternating Crystal Potential Comparison With Experiments on DMM-TCBQ ₂ . Molecular Crystals and Liquid Crystals, 1985, 120, 153-156.	0.8	4
46	Challenges for Industrial Ecology in Practice and Theory. Journal of Industrial Ecology, 2011, 15, 677-679.	5.5	2
47	Effect of Sulphur and Silicon in Fuels on an Automotive Reforming Catalyst. , 2005, , .		1
48	Risk Mitigation and Investability of a U-PHS Project in The Netherlands. Energies, 2020, 13, 5072.	3.1	1
49	A Worrier's Guide to the Future. Gaia, 2014, 23, 125-126.	0.7	0