Markus Kraft

List of Publications by Citations

344 papers	10,369 citations	53 h-index	86 g-index
360 ext. papers	11,965 ext. citations	6.1 avg, IF	6.85 L-index

#	Paper	IF	Citations
344	Blockchain technology in the chemical industry: Machine-to-machine electricity market. *Applied Energy*, **2017**, 195, 234-246	10.7	436
343	Nickel Nanoparticles Encapsulated in Few-Layer Nitrogen-Doped Graphene Derived from Metal-Organic Frameworks as Efficient Bifunctional Electrocatalysts for Overall Water Splitting. *Advanced Materials*, **2017**, 29, 1605957	24	421
342	Metal-free carbonaceous electrocatalysts and photocatalysts for water splitting. *Chemical Society Reviews*, **2016**, 45, 3039-52	58.5	419
341	Unique P?Co?N Surface Bonding States Constructed on g-C3N4 Nanosheets for Drastically Enhanced Photocatalytic Activity of H2 Evolution. *Advanced Functional Materials*, **2017**, 27, 1604328	15.6	266
340	Investigating the Role of Tunable Nitrogen Vacancies in Graphitic Carbon Nitride Nanosheets for Efficient Visible-Light-Driven H2 Evolution and CO2 Reduction. *ACS Sustainable Chemistry and Engineering*, **2017**, 5, 7260-7268	8.3	224
339	Measurement and numerical simulation of soot particle size distribution functions in a laminar premixed ethylene-oxygen-argon flame. *Combustion and Flame*, **2003**, 133, 173-188	5.3	208
338	Mapping surrogate gasoline compositions into RON/MON space. *Combustion and Flame*, **2010**, 157, 1122-1131	5.3	192
337	Incorporating seller/buyer reputation-based system in blockchain-enabled emission trading application. *Applied Energy*, **2018**, 209, 8-19	10.7	173
336	A Highly Efficient Oxygen Evolution Catalyst Consisting of Interconnected Nickel-Iron-Layered Double Hydroxide and Carbon Nanodomains. *Advanced Materials*, **2018**, 30, 1705106	24	153
335	Design of computer experiments: A review. *Computers and Chemical Engineering*, **2017**, 106, 71-95	4	132
334	Towards a detailed soot model for internal combustion engines. *Combustion and Flame*, **2009**, 156, 1156-1165	5.3	128
333	Numerical simulation and sensitivity analysis of detailed soot particle size distribution in laminar premixed ethylene flames. *Combustion and Flame*, **2006**, 145, 117-127	5.3	124
332	Modelling the internal structure of nascent soot particles. *Combustion and Flame*, **2010**, 157, 909-914	5.3	118
331	A quantitative study of the clustering of polycyclic aromatic hydrocarbons at high temperatures. *Physical Chemistry Chemical Physics*, **2012**, 14, 4081-94	3.6	117
330	Electronic and optical properties of aluminium-doped anatase and rutile TiO2 from ab initio calculations. *Physical Review B*, **2010**, 81,	3.3	115
329	A study on the coagulation of polycyclic aromatic hydrocarbon clusters to determine their collision efficiency. *Combustion and Flame*, **2010**, 157, 523-534	5.3	108
328	HRTEM evaluation of soot particles produced by the non-premixed combustion of liquid fuels. *Carbon*, **2016**, 96, 459-473	10.4	104

327	A statistical approach to develop a detailed soot growth model using PAH characteristics. *Combustion and Flame*, **2009**, 156, 896-913	5.3	104
326	Modelling soot formation in a premixed flame using an aromatic-site soot model and an improved oxidation rate. *Proceedings of the Combustion Institute*, **2009**, 32, 639-646	5.9	94
325	A new model for the drying of droplets containing suspended solids. *Chemical Engineering Science*, **2009**, 64, 628-637	4.4	94
324	Investigation of combustion emissions in a homogeneous charge compression injection engine: Measurements and a new computational model. *Proceedings of the Combustion Institute*, **2000**, 28, 1195-1201	5.9	93
323	Screening and techno-economic assessment of biomass-based power generation with CCS technologies to meet 2050 CO2 targets. *Applied Energy*, **2017**, 190, 481-489	10.7	90
322	Developing the PAH-PP soot particle model using process informatics and uncertainty propagation. *Proceedings of the Combustion Institute*, **2011**, 33, 675-683	5.9	88
321	Research advances towards large-scale solar hydrogen production from water. *EnergyChem*, **2019**, 1, 100014	36.9	82
320	The future viability of algae-derived biodiesel under economic and technical uncertainties. *Bioresource Technology*, **2014**, 151, 166-73	11	79
319	Numerical simulations of soot aggregation in premixed laminar flames. *Proceedings of the Combustion Institute*, **2007**, 31, 693-700	5.9	79
318	An Efficient Stochastic Algorithm for Simulating Nano-particle Dynamics. *Journal of Computational Physics*, **2002**, 183, 210-232	4.1	79
317	Stochastic modeling of soot particle size and age distributions in laminar premixed flames. *Proceedings of the Combustion Institute*, **2005**, 30, 1457-1465	5.9	75
316	Coupling a stochastic soot population balance to gas-phase chemistry using operator splitting. *Combustion and Flame*, **2007**, 148, 158-176	5.3	74
315	Quantitative tools for cultivating symbiosis in industrial parks; a literature review. *Applied Energy*, **2015**, 155, 599-612	10.7	71
314	A fully coupled simulation of PAH and soot growth with a population balance model. *Proceedings of the Combustion Institute*, **2013**, 34, 1827-1835	5.9	71
313	Models for the aggregate structure of soot particles. *Combustion and Flame*, **2007**, 151, 160-172	5.3	70
312	Modelling soot formation from wall films in a gasoline direct injection engine using a detailed population balance model. *Applied Energy*, **2016**, 163, 154-166	10.7	68
311	Applying Industry 4.0 to the Jurong Island Eco-industrial Park. *Energy Procedia*, **2015**, 75, 1536-1541	2.3	68
310	Aromatic site description of soot particles. *Combustion and Flame*, **2008**, 155, 161-180	5.3	68

309	The carbon footprint and non-renewable energy demand of algae-derived biodiesel. *Applied Energy* , **2014**, 113, 1632-1644	10.7	67
308	Toward a Comprehensive Model of the Synthesis of TiO2Particles from TiCl4. *Industrial & Engineering Chemistry Research*, **2007**, 46, 6147-6156	3.9	64
307	Simulating the structural evolution of droplets following shell formation. *Chemical Engineering Science*, **2010**, 65, 713-725	4.4	63
306	The Linear Process Deferment Algorithm: A new technique for solving population balance equations. *SIAM Journal of Scientific Computing*, **2006**, 28, 303-320	2.6	63
305	The evolution of the biofuel science. *Renewable and Sustainable Energy Reviews*, **2017**, 76, 1479-1484	16.2	62
304	First-principles thermochemistry for the production of TiO2 from TiCl4. *Journal of Physical Chemistry A*, **2007**, 111, 3560-5	2.8	62
303	A Detailed Model for the Sintering of Polydispersed Nanoparticle Agglomerates. *Aerosol Science and Technology*, **2009**, 43, 978-989	3.4	61
302	Detailed modeling of soot formation in a partially stirred plug flow reactor. *Combustion and Flame*, **2002**, 128, 395-409	5.3	61
301	Extending stochastic soot simulation to higher pressures. *Combustion and Flame*, **2006**, 145, 638-642	5.3	59
300	New polycyclic aromatic hydrocarbon (PAH) surface processes to improve the model prediction of the composition of combustion-generated PAHs and soot. *Carbon*, **2010**, 48, 319-332	10.4	58
299	A new numerical approach for the simulation of the growth of inorganic nanoparticles. *Journal of Computational Physics*, **2006**, 211, 638-658	4.1	58
298	A coupled CFD-population balance approach for nanoparticle synthesis in turbulent reacting flows. *Chemical Engineering Science*, **2011**, 66, 3792-3805	4.4	57
297	A new model for the drying of droplets containing suspended solids after shell formation. *Chemical Engineering Science*, **2009**, 64, 228-246	4.4	56
296	Parameter estimation in a multidimensional granulation model. *Powder Technology*, **2010**, 197, 196-210	5.2	56
295	PAH structure analysis of soot in a non-premixed flame using high-resolution transmission electron microscopy and optical band gap analysis. *Combustion and Flame*, **2016**, 164, 250-258	5.3	55
294	A First Principles Development of a General Anisotropic Potential for Polycyclic Aromatic Hydrocarbons. *Journal of Chemical Theory and Computation*, **2010**, 6, 683-95	6.4	55
293	Modelling the flame synthesis of silica nanoparticles from tetraethoxysilane. *Chemical Engineering Science*, **2012**, 70, 54-66	4.4	54
292	The simultaneous reduction of nitric oxide and soot in emissions from diesel engines. *Carbon*, **2009**, 47, 866-875	10.4	54

291	Sooting tendency of paraffin components of diesel and gasoline in diffusion flames. *Fuel*, **2014**, 126, 8-15	7.1	53
290	Modelling and validation of granulation with heterogeneous binder dispersion and chemical reaction. *Chemical Engineering Science*, **2007**, 62, 4717-4728	4.4	52
289	Modelling of a RDC using a combined CFD-population balance approach. *Chemical Engineering Science*, **2004**, 59, 2597-2606	4.4	51
288	Stochastic weighted particle methods for population balance equations. *Journal of Computational Physics*, **2011**, 230, 7456-7472	4.1	50
287	Internal structure of soot particles in a diffusion flame. *Carbon*, **2019**, 141, 635-642	10.4	50
286	Sooting tendency and particle size distributions of n-heptane/toluene mixtures burned in a wick-fed diffusion flame. *Fuel*, **2016**, 169, 111-119	7.1	49
285	Size-dependent melting of polycyclic aromatic hydrocarbon nano-clusters: A molecular dynamics study. *Carbon*, **2014**, 67, 79-91	10.4	49
284	Design technologies for eco-industrial parks: From unit operations to processes, plants and industrial networks. *Applied Energy*, **2016**, 175, 305-323	10.7	49
283	Numerical simulation and parametric sensitivity study of particle size distributions in a burner-stabilised stagnation flame. *Combustion and Flame*, **2015**, 162, 2569-2581	5.3	48
282	An improved methodology for determining threshold sooting indices from smoke point lamps. *Fuel* , **2013**, 111, 120-130	7.1	48
281	Techno-economic assessment of carbon-negative algal biodiesel for transport solutions. *Applied Energy*, **2013**, 106, 262-274	10.7	47
280	A mechanistic study on the simultaneous elimination of soot and nitric oxide from engine exhaust. *Carbon*, **2011**, 49, 1516-1531	10.4	47
279	Dual injection homogeneous charge compression ignition engine simulation using a stochastic reactor model. *International Journal of Engine Research*, **2007**, 8, 41-50	2.7	47
278	Sooting tendency of surrogates for the aromatic fractions of diesel and gasoline in a wick-fed diffusion flame. *Fuel*, **2015**, 153, 31-39	7.1	46
277	A detailed kinetic model for combustion synthesis of titania from TiCl4. *Combustion and Flame*, **2009**, 156, 1764-1770	5.3	45
276	Iterative improvement of Bayesian parameter estimates for an engine model by means of experimental design. *Combustion and Flame*, **2012**, 159, 1303-1313	5.3	43
275	Smart Sampling Algorithm for Surrogate Model Development. *Computers and Chemical Engineering*, **2017**, 96, 103-114	4	41
274	Real-Time Evaluation of a Detailed Chemistry HCCI Engine Model Using a Tabulation Technique. *Combustion Science and Technology*, **2008**, 180, 1263-1277	1.5	41

273	The Polarization of Polycyclic Aromatic Hydrocarbons Curved by Pentagon Incorporation: The Role of the Flexoelectric Dipole. *Journal of Physical Chemistry C*, **2017**, 121, 27154-27163	3.8	40
272	A multidimensional population balance model to describe the aerosol synthesis of silica nanoparticles. *Journal of Aerosol Science*, **2012**, 44, 83-98	4.3	40
271	Influence of Injection Timing and Piston Bowl Geometry on PCCI Combustion and Emissions. *SAE International Journal of Engines*, **2009**, 2, 1019-1033	2.4	40
270	A computational study of an HCCI engine with direct injection during gas exchange. *Combustion and Flame*, **2006**, 147, 118-132	5.3	40
269	The impact of intelligent cyber-physical systems on the decarbonization of energy. *Energy and Environmental Science*, **2020**, 13, 744-771	35.4	39
268	Sources of CO emissions in an HCCI engine: A numerical analysis. *Combustion and Flame*, **2006**, 144, 634-637	5.3	39
267	Sooting characteristics of polyoxymethylene dimethyl ether blends with diesel in a diffusion flame. *Fuel*, **2018**, 224, 499-506	7.1	38
266	Numerical investigation of DQMoM-IEM as a turbulent reaction closure. *Chemical Engineering Science*, **2010**, 65, 1915-1924	4.4	38
265	Homogeneous Charge Compression Ignition Engine: A Simulation Study on the Effects of Inhomogeneities. *Journal of Engineering for Gas Turbines and Power*, **2003**, 125, 466-471	1.7	37
264	Stochastic weighted particle methods for population balance equations with coagulation, fragmentation and spatial inhomogeneity. *Journal of Computational Physics*, **2015**, 303, 1-18	4.1	34
263	First-principles thermochemistry for silicon species in the decomposition of tetraethoxysilane. *Journal of Physical Chemistry A*, **2009**, 113, 9041-9	2.8	34
262	A novel methodology for the design of waste heat recovery network in eco-industrial park using techno-economic analysis and multi-objective optimization. *Applied Energy*, **2016**, 184, 88-102	10.7	34
261	Modelling soot formation in a DISI engine. *Proceedings of the Combustion Institute*, **2011**, 33, 3159-3167	5.9	33
260	Knowledge management of eco-industrial park for efficient energy utilization through ontology-based approach. *Applied Energy*, **2017**, 204, 1412-1421	10.7	32
259	Droplets population balance in a rotating disc contactor: An inverse problem approach. *AICHE Journal*, **2006**, 52, 1441-1450	3.6	32
258	Simulation of coalescence and breakage: an assessment of two stochastic methods suitable for simulating liquid□quid extraction. *Chemical Engineering Science*, **2004**, 59, 3865-3881	4.4	32
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256	Evaluating the EGR-AFR Operating Range of a HCCI Engine **2005**,		32

255	On a multivariate population balance model to describe the structure and composition of silica nanoparticles. *Computers and Chemical Engineering*, **2012**, 43, 130-147	4	31
254	Reactivity of Polycyclic Aromatic Hydrocarbon Soot Precursors: Implications of Localized Radicals on Rim-Based Pentagonal Rings. *Journal of Physical Chemistry C*, **2019**, 123, 26673-26682	3.8	30
253	An ontology framework towards decentralized information management for eco-industrial parks. *Computers and Chemical Engineering*, **2018**, 118, 49-63	4	30
252	Soot particle size distributions in premixed stretch-stabilized flat ethylene–oxygen–argon flames. *Proceedings of the Combustion Institute*, **2017**, 36, 1001-1009	5.9	30
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250	Stochastic solution of population balance equations for reactor networks. *Journal of Computational Physics*, **2014**, 256, 615-629	4.1	29
249	First-Principles Thermochemistry for the Thermal Decomposition of Titanium Tetraisopropoxide. *Journal of Physical Chemistry A*, **2015**, 119, 8376-87	2.8	28
248	Statistical Approximation of the Inverse Problem in Multivariate Population Balance Modeling. *Industrial & Engineering Chemistry Research*, **2010**, 49, 428-438	3.9	28
247	Numerical study of a stochastic particle algorithm solving a multidimensional population balance model for high shear granulation. *Journal of Computational Physics*, **2010**, 229, 7672-7691	4.1	28
246	Polymorphism of nanocrystalline TiO prepared in a stagnation flame: formation of the TiO-II phase. *Chemical Science*, **2019**, 10, 1342-1350	9.4	27
245	Modelling soot formation in a benchmark ethylene stagnation flame with a new detailed population balance model. *Combustion and Flame*, **2019**, 203, 56-71	5.3	27
244	Polar curved polycyclic aromatic hydrocarbons in soot formation. *Proceedings of the Combustion Institute*, **2019**, 37, 1117-1123	5.9	27
243	J-Park Simulator: An ontology-based platform for cross-domain scenarios in process industry. *Computers and Chemical Engineering*, **2019**, 131, 106586	4	27
242	Simulation and life cycle assessment of algae gasification process in dual fluidized bed gasifiers. *Green Chemistry*, **2015**, 17, 1793-1801	10	27
241	Incorporating experimental uncertainties into multivariate granulation modelling. *Chemical Engineering Science*, **2010**, 65, 1088-1100	4.4	27
240	OntoKin: An Ontology for Chemical Kinetic Reaction Mechanisms. *Journal of Chemical Information and Modeling*, **2020**, 60, 108-120	6.1	27
239	A new model for silicon nanoparticle synthesis. *Combustion and Flame*, **2013**, 160, 947-958	5.3	26
238	Giant fullerene formation through thermal treatment of fullerene soot. *Carbon*, **2017**, 125, 132-138	10.4	26

237	Bayesian Error Propagation for a Kinetic Model of n-Propylbenzene Oxidation in a Shock Tube. *International Journal of Chemical Kinetics*, **2014**, 46, 389-404	1.4	26
236	A Monte Carlo methods for identification and sensitivity analysis of coagulation processes. *Journal of Computational Physics*, **2004**, 200, 50-59	4.1	26
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234	A transferable electrostatic model for intermolecular interactions between polycyclic aromatic hydrocarbons. *Chemical Physics Letters*, **2011**, 510, 154-160	2.5	25
233	The inverse problem in granulation modeling□wo different statistical approaches. *AICHE Journal*, **2011**, 57, 3105-3121	3.6	25
232	The future of computational modelling in reaction engineering. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2010**, 368, 3633-44	3	25
231	Modelling nanoparticle dynamics: coagulation, sintering, particle inception and surface growth. *Combustion Theory and Modelling*, **2005**, 9, 449-461	1.5	25
230	Modelling particle mass and particle number emissions during the active regeneration of diesel particulate filters. *Proceedings of the Combustion Institute*, **2019**, 37, 4831-4838	5.9	25
229	LEAPS2: Learning based Evolutionary Assistive Paradigm for Surrogate Selection. *Computers and Chemical Engineering*, **2018**, 119, 352-370	4	25
228	Towards an ontological infrastructure for chemical process simulation and optimization in the context of eco-industrial parks. *Applied Energy*, **2017**, 204, 1284-1298	10.7	24
227	Modelling PAH curvature in laminar premixed flames using a detailed population balance model. *Combustion and Flame*, **2017**, 176, 172-180	5.3	24
226	Phase change of polycyclic aromatic hydrocarbon clusters by mass addition. *Carbon*, **2014**, 77, 25-35	10.4	24
225	Adsorption, diffusion and desorption of chlorine on and from rutile TiO2{110}: a theoretical investigation. *ChemPhysChem*, **2007**, 8, 444-51	3.2	24
224	Modelling a Dual-Fuelled Multi-Cylinder HCCI Engine Using a PDF Based Engine Cycle Simulator **2004**,		24
223	Extension of moment projection method to the fragmentation process. *Journal of Computational Physics*, **2017**, 335, 516-534	4.1	23
222	Partially Stirred Reactor Model: Analytical Solutions and Numerical Convergence Study of a PDF/Monte Carlo Method. *SIAM Journal of Scientific Computing*, **2004**, 25, 1798-1823	2.6	23
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220	Modelling TiO 2 formation in a stagnation flame using method of moments with interpolative closure. *Combustion and Flame*, **2017**, 178, 135-147	5.3	22

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218	Investigation of the impact of the configuration of exhaust after-treatment system for diesel engines. *Applied Energy*, **2020**, 267, 114844	10.7	22
217	Numerical simulation and parametric sensitivity study of optical band gap in a laminar co-flow ethylene diffusion flame. *Combustion and Flame*, **2016**, 167, 320-334	5.3	22
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215	Particle Formation and Models **2014**, 1-23		22
214	First-principles thermochemistry for the combustion of a TiCl4 and AlCl3 mixture. *Journal of Physical Chemistry A*, **2009**, 113, 13790-6	2.8	22
213	Comparison of the stochastic fields method and DQMoM-IEM as turbulent reaction closures. *Chemical Engineering Science*, **2010**, 65, 5429-5441	4.4	22
212	Simulating a Homogeneous Charge Compression Ignition Engine Fuelled with a DEE/EtOH Blend **2006**,		22
211	Development of a multi-compartment population balance model for high-shear wet granulation with discrete element method. *Computers and Chemical Engineering*, **2017**, 99, 171-184	4	21
210	Optimal site selection for modular nuclear power plants. *Computers and Chemical Engineering*, **2019**, 125, 339-350	4	21
209	Experimental and numerical study of the evolution of soot primary particles in a diffusion flame. *Proceedings of the Combustion Institute*, **2019**, 37, 2047-2055	5.9	21
208	Bayesian parameter estimation for a jet-milling model using Metropolis□Hastings and Wang□Landau sampling. *Chemical Engineering Science*, **2013**, 89, 244-257	4.4	21
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206	Improved methodology for performing the inverse Abel transform of flame images for color ratio pyrometry. *Applied Optics*, **2019**, 58, 2662-2670	1.7	21
205	Topology of Disordered 3D Graphene Networks. *Physical Review Letters*, **2019**, 123, 116105	7.4	20
204	An Ontology and Semantic Web Service for Quantum Chemistry Calculations. *Journal of Chemical Information and Modeling*, **2019**, 59, 3154-3165	6.1	20
203	Microkinetic Modeling of the Fischer□Tropsch Synthesis over Cobalt Catalysts. *ChemCatChem*, **2015**, 7, 137-143	5.2	20
202	OntoPowSys: A power system ontology for cross domain interactions in an eco industrial park. *Energy and AI*, **2020**, 1, 100008	12.6	20

201	Optical band gap of cross-linked, curved, and radical polyaromatic hydrocarbons. *Physical Chemistry Chemical Physics*, **2019**, 21, 16240-16251	3.6	20
200	Surface reactivity of polycyclic aromatic hydrocarbon clusters. *Proceedings of the Combustion Institute*, **2015**, 35, 1811-1818	5.9	20
199	Theoretical insights into the surface growth of rutile TiO2. *Combustion and Flame*, **2011**, 158, 1868-1876	5.3	20
198	Assessing the polycyclic aromatic hydrocarbon anisotropic potential with application to the exfoliation energy of graphite. *Journal of Physical Chemistry A*, **2011**, 115, 13684-93	2.8	20
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193	Premixed Stagnation Flame Synthesized TiO2 Nanoparticles with Mixed Phases for Efficient Photocatalytic Hydrogen Generation. *ACS Sustainable Chemistry and Engineering*, **2018**, 6, 14470-14479	8.3	19
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191	Box-Behnken design based CO2 co-gasification of horticultural waste and sewage sludge with addition of ash from waste as catalyst. *Applied Energy*, **2019**, 242, 1549-1561	10.7	18
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182	Soot inception: Carbonaceous nanoparticle formation in flames. *Progress in Energy and Combustion Science*, **2022**, 88, 100956	33.6	17
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178	Modelling gas-phase synthesis of single-walled carbon nanotubes on iron catalyst particles. *Carbon*, **2008**, 46, 422-433	10.4	16
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174	Direct Simulation and Mass Flow Stochastic Algorithms to Solve a Sintering-Coagulation Equation. *Monte Carlo Methods and Applications*, **2005**, 11,	0.4	15
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166	Game theory-based renewable multi-energy system design and subsidy strategy optimization. *Advances in Applied Energy*, **2021**, 2, 100024		14

165	Partitioning of polycyclic aromatic hydrocarbons in heterogeneous clusters. *Carbon*, **2019**, 143, 247-256	10.4	14
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