A Rabdel Ruiz-Salvador

List of Publications by Year
in descending order

56 papers	2,215 citations	218677 26 h-index	214800 47 g-index
58 all docs	58 docs citations	58 times ranked	2978 citing authors

#	Article	IF	Citations
1	Zeolitic Polyoxometalate-Based Metalâ^'Organic Frameworks (Z-POMOFs): Computational Evaluation of Hypothetical Polymorphs and the Successful Targeted Synthesis of the Redox-Active Z-POMOF1. Journal of the American Chemical Society, 2009, 131, 16078-16087.	13.7	265
2	Zeolitic imidazole frameworks: structural and energetics trends compared with their zeolite analogues. CrystEngComm, 2009, 11, 2272.	2.6	217
3	Selective sulfur dioxide adsorption on crystal defect sites on an isoreticular metal organic framework series. Nature Communications, 2017, 8, 14457.	12.8	133
4	Step-wise dealumination of natural clinoptilolite: Structural and physicochemical characterization. Microporous and Mesoporous Materials, 2010, 135, 187-196.	4.4	129
5	Porphyrin-based metal-organic frameworks for solar fuel synthesis photocatalysis: band gap tuning via iron substitutions. Journal of Materials Chemistry A, 2017, 5, 11894-11904.	10.3	84
6	An Elementary Picture of Dielectric Spectroscopy in Solids: Physical Basis. Journal of Chemical Education, 2003, 80, 1062.	2.3	77
7	Chemical Engineering of Photoactivity in Heterometallic Titaniumâ€“Organic Frameworks by Metal Doping. Angewandte Chemie - International Edition, 2018, 57, 8453-8457.	13.8	72
8	Modelling a Linker Mixâ€andâ€Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. Angewandte Chemie - International Edition, 2016, 55, 16012-16016.	13.8	61
9	Electronic structure of porphyrin-based metalâ€“organic frameworks and their suitability for solar fuel production photocatalysis. Journal of Materials Chemistry A, 2015, 3, 23458-23465.	10.3	59
10	Tuning the separation properties of zeolitic imidazolate framework coreâ€“shell structures via post-synthetic modification. Journal of Materials Chemistry A, 2017, 5, 25601-25608.	10.3	56
11	Interaction studies between drugs and a purified natural clinoptilolite. Microporous and Mesoporous Materials, 2003, 61, 117-125.	4.4	55
12	Zeolitic polyoxometalates metal organic frameworks (Z-POMOF) with imidazole ligands and Îµ-Keggin ions as building blocks; computational evaluation of hypothetical polymorphs and a synthesis approach. Physical Chemistry Chemical Physics, 2010, 12, 8632.	2.8	51
13	Thermal and cation influence on ir vibrations of modified natural clinoptilolite. Microporous and Mesoporous Materials, 1998, 20, 269-281.	4.4	50
14	Preliminary characterization of drug support systems based on natural clinoptilolite. Microporous and Mesoporous Materials, 2003, 61, 249-259.	4.4	49
15	A computer simulation study of distribution, structure and acid strength of active sites in H-ZSM-5 catalyst. Physical Chemistry Chemical Physics, 2000, 2, 5716-5722.	2.8	47
16	Îµ-Keggin-based coordination networks: Synthesis, structure and application toward green synthesis of polyoxometalate@graphene hybrids. Dalton Transactions, 2012, 41, 9989.	3.3	47
17	Atomic charges for modeling metalâ€“organic frameworks: Why and how. Journal of Solid State Chemistry, 2015, 223, 144-151.	2.9	47
18	Understanding Nanopore Window Distortions in the Reversible Molecular Valve Zeolite RHO. Chemistry of Materials, 2015, 27, 5657-5667.	6.7	42

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19	Controlling Thermal Expansion: A Metalâ€“Organic Frameworks Route. Chemistry of Materials, 2016, 28, 8296-8304.	6.7	42
20	Aluminum Distribution in Low Si/Al Zeolites:â€‰ Dehydrated Naâ^'Clinoptilolite. Journal of Physical Chemistry B, 1998, 102, 8417-8425.	2.6	41
21	Thermochemistry of strontium incorporation in aragonite from atomistic simulations. Geochimica Et Cosmochimica Acta, 2010, 74, 1320-1328.	3.9	34
22	The Siâ€“Ge substitutional series in the chiral STW zeolite structure type. Journal of Materials Chemistry A, 2018, 6, 15110-15122.	10.3	33
23	CeO2 thin films by flash evaporation. Solid State Ionics, 1997, 96, 89-93.	2.7	32
24	Space group symmetry and Alâ€”Oâ€”P bond angles in AlPO4-5. Journal of Materials Chemistry, 1996, 6, 1837-1842.	6.7	31
25	Clinoptiloliteâ€“heulandite polymorphism: structural features from computer simulation. Physical Chemistry Chemical Physics, 2000, 2, 1803-1813.	2.8	28
26	A free energy minimisation study of the monoclinicâ€“orthorhombic transition in MFI zeolite. Chemical Communications, 2002, , 2544-2545.	4.1	28
27	Pressure-Induced Hydration Effects in the Zeolite Laumontite. Angewandte Chemie - International Edition, 2004, 43, 469-472.	13.8	26
28	Comparing gas separation performance between all known zeolites and their zeolitic imidazolate framework counterparts. Dalton Transactions, 2016, 45, 216-225.	3.3	26
29	Modelling of hydrated Ca-rich zeolites. Molecular Simulation, 2002, 28, 649-661.	2.0	24
30	Surprising role of the BDC organic ligand in the adsorption of CO2 by MOF-5. Microporous and Mesoporous Materials, 2012, 163, 186-191.	4.4	24
31	Understanding Si/Al distributions in Al-rich zeolites: the role of water in determining the structure of Goosecreekite. Chemical Communications, 2001, , 531-532.	4.1	23
32	Siliconâ€“aluminium distribution in dehydrated calcium heulandite. Physical Chemistry Chemical Physics, 1999, 1, 1679-1685.	2.8	22
33	Critical Role of Dynamic Flexibility in Geâ€Containing Zeolites: Impact on Diffusion. Chemistry - A European Journal, 2016, 22, 10036-10043.	3.3	22
34	Interplay of water, extra-framework cations and framework atoms in the structure of low-silicazeolites: the case of the natural zeolite Goosecreekite as studied by computer simulation. Physical Chemistry Chemical Physics, 2007, 9, 521-532.	2.8	21
35	Aluminium distribution in ZSM-5 revisited: The role of Alâ€“Al interactions. Journal of Solid State Chemistry, 2013, 198, 330-336.	2.9	21
36	Conductivity activation energy and analysis of the sintering process of dielectric ceramics. Materials Letters, 1998, 36, 290-293.	2.6	20

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37	Computational study of substitution of Al by Fe3+ in the AlPO4-5 framework. Microporous and Mesoporous Materials, 1999, 29, 361-367.	4.4	20
38	Location of extra-framework Co2+, Ni2+, Cu2+ and Zn2+ cations in natural and dealuminated clinoptilolite. Microporous and Mesoporous Materials, 2012, 155, 233-239.	4.4	19
39	Preparation of natural zeolitic supports for potential biomedical applications. Materials Chemistry and Physics, 2009, 118, 322-328.	4.0	18
40	Importance of Blocking Inaccessible Voids on Modeling Zeolite Adsorption: Revisited. Journal of Physical Chemistry C, 2017, 121, 4462-4470.	3.1	17
41	Thermostructural behaviour of Niâ€“Cr materials: modelling of bulk and nanoparticle systems. Physical Chemistry Chemical Physics, 2015, 17, 15912-15920.	2.8	13
42	A DFT-based simulated annealing method for the optimization of global energy in zeolite framework systems: Application to natrolite, chabazite and clinoptilolite. Microporous and Mesoporous Materials, 2020, 294, 109885.	4.4	13
43	Modelling a Linker Mixâ€andâ€Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. Angewandte Chemie, 2016, 128, 16246-16250.	2.0	12
44	Locating Extra-Framework Cations in Low-Silica Zeolites by a Combinatorial Approach of the Direct Space Method and Rietveld Refinement: Application to Ni2+ and Co2+ Enriched Clinoptilolite. Journal of Physical Chemistry C, 2010, 114, 5964-5974.	3.1	10
45	Mg/Ca Partitioning Between Aqueous Solution and Aragonite Mineral: A Molecular Dynamics Study. Chemistry - A European Journal, 2012, 18, 9828-9833.	3.3	10
46	Chemical Engineering of Photoactivity in Heterometallic Titaniumâ€“Organic Frameworks by Metal Doping. Angewandte Chemie, 2018, 130, 8589-8593.	2.0	9
47	Si atoms in SAPO-31: A computational study. Studies in Surface Science and Catalysis, 2004, 154, 1439-1447.	1.5	5
48	Separation of electronic and ionic conductivity in mixed conductors from the ac response: Application to Pr0.56Bi0.04Li0.2TiO3. Applied Physics Letters, 2008, 93, 034105.	3.3	5
49	Proton mobility calculations in the presence of negative capacitances. Europhysics Letters, 1998, 44, 211-215.	2.0	3
50	Approaching the structure of heavily defective ionic oxides through atomistic modeling. Physica Status Solidi C: Current Topics in Solid State Physics, 2005, 2, 3521-3524.	0.8	3
51	Screening heteroatom distributions in zeotype materials using an effective Hamiltonian approach: the case of aluminogermanate PKU-9. Physical Chemistry Chemical Physics, 2018, 20, 18047-18055.	2.8	3
52	Unravelling the key factors in the chlorine-promoted epoxidation of ethylene over a silverâ€“copper oxide nanocatalyst. Nanoscale, 2022, 14, 7332-7340.	5.6	3
53	Reactivity Analysis in Diamond Surfaces with a Density Functional Calculation. Structural Chemistry, 2001, 12, 101-111.	2.0	2
54	Chemical insertion in the perovskite solid solutions Pr0.5+xâ”yLi0.5â”3xBiyâ–¡2xTiO3: Implications on the electrical properties. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2012, 177, 563-569.	3.5	2

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55	Fitting electron density as a physically sound basis for the development of interatomic potentials of complex alloys. Physical Chemistry Chemical Physics, 2018, 20, 18647-18656.	2.8	2
56	Thermostructural Characterization of Silicon Carbide Nanocomposite Materials via Molecular Dynamics Simulations. Advanced Composite Materials, 2022, 31, 485-504.	1.9	0