

# A Rabdel Ruiz-Salvador

## List of Publications by Year in descending order

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56  
papers

2,215  
citations

218677

26  
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214800

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58  
all docs

58  
docs citations

58  
times ranked

2978  
citing authors

#	ARTICLE	IF	CITATIONS
1	Thermostructural Characterization of Silicon Carbide Nanocomposite Materials via Molecular Dynamics Simulations. <i>Advanced Composite Materials</i> , 2022, 31, 485-504.	1.9	0
2	Unravelling the key factors in the chlorine-promoted epoxidation of ethylene over a silver-copper oxide nanocatalyst. <i>Nanoscale</i> , 2022, 14, 7332-7340.	5.6	3
3	A DFT-based simulated annealing method for the optimization of global energy in zeolite framework systems: Application to natrolite, chabazite and clinoptilolite. <i>Microporous and Mesoporous Materials</i> , 2020, 294, 109885.	4.4	13
4	The Si-Ge substitutional series in the chiral STW zeolite structure type. <i>Journal of Materials Chemistry A</i> , 2018, 6, 15110-15122.	10.3	33
5	Screening heteroatom distributions in zeotype materials using an effective Hamiltonian approach: the case of aluminogermanate PKU-9. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 18047-18055.	2.8	3
6	Chemical Engineering of Photoactivity in Heterometallic Titanium-Organic Frameworks by Metal Doping. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 8453-8457.	13.8	72
7	Chemical Engineering of Photoactivity in Heterometallic Titanium-Organic Frameworks by Metal Doping. <i>Angewandte Chemie</i> , 2018, 130, 8589-8593.	2.0	9
8	Fitting electron density as a physically sound basis for the development of interatomic potentials of complex alloys. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 18647-18656.	2.8	2
9	Importance of Blocking Inaccessible Voids on Modeling Zeolite Adsorption: Revisited. <i>Journal of Physical Chemistry C</i> , 2017, 121, 4462-4470.	3.1	17
10	Selective sulfur dioxide adsorption on crystal defect sites on an isorecticular metal organic framework series. <i>Nature Communications</i> , 2017, 8, 14457.	12.8	133
11	Porphyrim-based metal-organic frameworks for solar fuel synthesis photocatalysis: band gap tuning via iron substitutions. <i>Journal of Materials Chemistry A</i> , 2017, 5, 11894-11904.	10.3	84
12	Tuning the separation properties of zeolitic imidazolate framework core-shell structures via post-synthetic modification. <i>Journal of Materials Chemistry A</i> , 2017, 5, 25601-25608.	10.3	56
13	Critical Role of Dynamic Flexibility in Ge-Containing Zeolites: Impact on Diffusion. <i>Chemistry - A European Journal</i> , 2016, 22, 10036-10043.	3.3	22
14	Modelling a Linker Mix-and-Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 16012-16016.	13.8	61
15	Modelling a Linker Mix-and-Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. <i>Angewandte Chemie</i> , 2016, 128, 16246-16250.	2.0	12
16	Controlling Thermal Expansion: A Metal-Organic Frameworks Route. <i>Chemistry of Materials</i> , 2016, 28, 8296-8304.	6.7	42
17	Comparing gas separation performance between all known zeolites and their zeolitic imidazolate framework counterparts. <i>Dalton Transactions</i> , 2016, 45, 216-225.	3.3	26
18	Thermostructural behaviour of Ni-Cr materials: modelling of bulk and nanoparticle systems. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 15912-15920.	2.8	13

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19	Understanding Nanopore Window Distortions in the Reversible Molecular Valve Zeolite RHO. <i>Chemistry of Materials</i> , 2015, 27, 5657-5667.	6.7	42
20	Electronic structure of porphyrin-based metal-organic frameworks and their suitability for solar fuel production photocatalysis. <i>Journal of Materials Chemistry A</i> , 2015, 3, 23458-23465.	10.3	59
21	Atomic charges for modeling metal-organic frameworks: Why and how. <i>Journal of Solid State Chemistry</i> , 2015, 223, 144-151.	2.9	47
22	Aluminium distribution in ZSM-5 revisited: The role of Al-Al interactions. <i>Journal of Solid State Chemistry</i> , 2013, 198, 330-336.	2.9	21
23	Surprising role of the BDC organic ligand in the adsorption of CO <sub>2</sub> by MOF-5. <i>Microporous and Mesoporous Materials</i> , 2012, 163, 186-191.	4.4	24
24	μ-Keggin-based coordination networks: Synthesis, structure and application toward green synthesis of polyoxometalate-graphene hybrids. <i>Dalton Transactions</i> , 2012, 41, 9989.	3.3	47
25	Mg/Ca Partitioning Between Aqueous Solution and Aragonite Mineral: A Molecular Dynamics Study. <i>Chemistry - A European Journal</i> , 2012, 18, 9828-9833.	3.3	10
26	Location of extra-framework Co <sup>2+</sup> , Ni <sup>2+</sup> , Cu <sup>2+</sup> and Zn <sup>2+</sup> cations in natural and dealuminated clinoptilolite. <i>Microporous and Mesoporous Materials</i> , 2012, 155, 233-239.	4.4	19
27	Chemical insertion in the perovskite solid solutions Pr <sub>0.5</sub> xLi <sub>0.5</sub> 3xBiy- <sub>2</sub> TiO <sub>3</sub> : Implications on the electrical properties. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2012, 177, 563-569.	3.5	2
28	Step-wise dealumination of natural clinoptilolite: Structural and physicochemical characterization. <i>Microporous and Mesoporous Materials</i> , 2010, 135, 187-196.	4.4	129
29	Zeolitic polyoxometalates metal organic frameworks (Z-POMOF) with imidazole ligands and μ-Keggin ions as building blocks; computational evaluation of hypothetical polymorphs and a synthesis approach. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 8632.	2.8	51
30	Thermochemistry of strontium incorporation in aragonite from atomistic simulations. <i>Geochimica Et Cosmochimica Acta</i> , 2010, 74, 1320-1328.	3.9	34
31	Locating Extra-Framework Cations in Low-Silica Zeolites by a Combinatorial Approach of the Direct Space Method and Rietveld Refinement: Application to Ni <sup>2+</sup> and Co <sup>2+</sup> Enriched Clinoptilolite. <i>Journal of Physical Chemistry C</i> , 2010, 114, 5964-5974.	3.1	10
32	Preparation of natural zeolitic supports for potential biomedical applications. <i>Materials Chemistry and Physics</i> , 2009, 118, 322-328.	4.0	18
33	Zeolitic imidazole frameworks: structural and energetics trends compared with their zeolite analogues. <i>CrystEngComm</i> , 2009, 11, 2272.	2.6	217
34	Zeolitic Polyoxometalate-Based Metal-Organic Frameworks (Z-POMOFs): Computational Evaluation of Hypothetical Polymorphs and the Successful Targeted Synthesis of the Redox-Active Z-POMOF1. <i>Journal of the American Chemical Society</i> , 2009, 131, 16078-16087.	13.7	265
35	Separation of electronic and ionic conductivity in mixed conductors from the ac response: Application to Pr <sub>0.56</sub> Bi <sub>0.04</sub> Li <sub>0.2</sub> TiO <sub>3</sub> . <i>Applied Physics Letters</i> , 2008, 93, 034105.	3.3	5
36	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. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 521-532.	2.8	21

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37	Approaching the structure of heavily defective ionic oxides through atomistic modeling. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2005, 2, 3521-3524.	0.8	3
38	Si atoms in SAPO-31: A computational study. <i>Studies in Surface Science and Catalysis</i> , 2004, 154, 1439-1447.	1.5	5
39	Pressure-Induced Hydration Effects in the Zeolite Laumontite. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 469-472.	13.8	26
40	Preliminary characterization of drug support systems based on natural clinoptilolite. <i>Microporous and Mesoporous Materials</i> , 2003, 61, 249-259.	4.4	49
41	Interaction studies between drugs and a purified natural clinoptilolite. <i>Microporous and Mesoporous Materials</i> , 2003, 61, 117-125.	4.4	55
42	An Elementary Picture of Dielectric Spectroscopy in Solids: Physical Basis. <i>Journal of Chemical Education</i> , 2003, 80, 1062.	2.3	77
43	Modelling of hydrated Ca-rich zeolites. <i>Molecular Simulation</i> , 2002, 28, 649-661.	2.0	24
44	A free energy minimisation study of the monoclinic $\leftrightarrow$ orthorhombic transition in MFI zeolite. <i>Chemical Communications</i> , 2002, , 2544-2545.	4.1	28
45	Understanding Si/Al distributions in Al-rich zeolites: the role of water in determining the structure of Goosecreekite. <i>Chemical Communications</i> , 2001, , 531-532.	4.1	23
46	Reactivity Analysis in Diamond Surfaces with a Density Functional Calculation. <i>Structural Chemistry</i> , 2001, 12, 101-111.	2.0	2
47	Clinoptilolite $\leftrightarrow$ heulandite polymorphism: structural features from computer simulation. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 1803-1813.	2.8	28
48	A computer simulation study of distribution, structure and acid strength of active sites in H-ZSM-5 catalyst. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 5716-5722.	2.8	47
49	Computational study of substitution of Al by Fe <sup>3+</sup> in the AlPO <sub>4</sub> -5 framework. <i>Microporous and Mesoporous Materials</i> , 1999, 29, 361-367.	4.4	20
50	Silicon $\leftrightarrow$ aluminium distribution in dehydrated calcium heulandite. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 1679-1685.	2.8	22
51	Thermal and cation influence on ir vibrations of modified natural clinoptilolite. <i>Microporous and Mesoporous Materials</i> , 1998, 20, 269-281.	4.4	50
52	Conductivity activation energy and analysis of the sintering process of dielectric ceramics. <i>Materials Letters</i> , 1998, 36, 290-293.	2.6	20
53	Aluminum Distribution in Low Si/Al Zeolites: Dehydrated Na <sup>+</sup> Clinoptilolite. <i>Journal of Physical Chemistry B</i> , 1998, 102, 8417-8425.	2.6	41
54	Proton mobility calculations in the presence of negative capacitances. <i>Europhysics Letters</i> , 1998, 44, 211-215.	2.0	3

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55	CeO <sub>2</sub> thin films by flash evaporation. <i>Solid State Ionics</i> , 1997, 96, 89-93.	2.7	32
56	Space group symmetry and Al-O-P bond angles in AlPO <sub>4</sub> -5. <i>Journal of Materials Chemistry</i> , 1996, 6, 1837-1842.	6.7	31