Jose M Vicent-Luna

List of Publications by Year
in descending order

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52	1,261	331538	395590
papers	citations	21 h-index	33 g-index

54	54	54	1718
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Transitioning from Ionic Liquids to Deep Eutectic Solvents. ACS Sustainable Chemistry and Engineering, 2022, 10, 1232-1245.	3.2	22
2	Adsorption of Linear Alcohols in Amorphous Activated Carbons: Implications for Energy Storage Applications. ACS Sustainable Chemistry and Engineering, 2022, 10, 6509-6520.	3.2	5
3	Transferable Classical Force Field for Pure and Mixed Metal Halide Perovskites Parameterized from First-Principles. Journal of Chemical Information and Modeling, 2022, 62, 6423-6435.	2.5	5
4	Refined GFN1-xTB Parameters for Engineering Phase-Stable CsPbX₃ Perovskites. Journal of Physical Chemistry C, 2022, 126, 9587-9596.	1.5	2
5	Phase transformation barrier modulation of CsPbI3 films via PbI3â˜ complex for efficient all-inorganic perovskite photovoltaics. Nano Energy, 2022, 99, 107388.	8.2	9
6	Enhancing separation efficiency in European syngas industry by using zeolites. Catalysis Today, 2021, 362, 113-121.	2.2	10
7	Waterâ€“Gas Shift Reaction to Capture Carbon Dioxide and Separate Hydrogen on Single-Walled Carbon Nanotubes. ACS Applied Materials & Interfaces, 2021, 13, 11026-11038.	4.0	10
8	Atomistic Insights Into the Degradation of Inorganic Halide Perovskite CsPbI₃: A Reactive Force Field Molecular Dynamics Study. Journal of Physical Chemistry Letters, 2021, 12, 5519-5525.	2.1	31
9	Efficient Computation of Structural and Electronic Properties of Halide Perovskites Using Density Functional Tight Binding: GFN1-xTB Method. Journal of Chemical Information and Modeling, 2021, 61, 4415-4424.	2.5	16
10	EMIMBF4 in ternary liquid mixtures of water, dimethyl sulfoxide and acetonitrile as â€œtri-solvent-in-saltâ€•electrolytes for high-performance supercapacitors operating at -70ÂÂ°C. Energy Storage Materials, 2021, 40, 368-385.	9.5	25
11	Effect of Coâ€Solvents on the Crystallization and Phase Distribution of Mixedâ€Dimensional Perovskites. Advanced Energy Materials, 2021, 11, 2102144.	10.2	25
12	Effect of Coâ€Solvents on the Crystallization and Phase Distribution of Mixedâ€Dimensional Perovskites (Adv. Energy Mater. 42/2021). Advanced Energy Materials, 2021, 11, 2170168.	10.2	0
13	Ï€-Complexation for olefin/paraffin separation using aluminosilicates. Chemical Engineering Journal, 2020, 380, 122482.	6.6	28
14	Role of hydrogen bonding in the capture and storage of ammonia in zeolites. Chemical Engineering Journal, 2020, 387, 124062.	6.6	37
15	Aqueous Coâ€Solvent in Zwitterionicâ€based Protic Ionic Liquids as Electrolytes in 2.0â€…V Supercapacitors. ChemSusChem, 2020, 13, 5983-5995.	3.6	8
16	Exploiting the Ï€-bonding for the separation of benzene and cyclohexane in zeolites. Chemical Engineering Journal, 2020, 398, 125678.	6.6	23
17	Efficient modelling of ion structure and dynamics in inorganic metal halide perovskites. Journal of Materials Chemistry A, 2020, 8, 11824-11836.	5.2	26
18	Further Extending the Dilution Range of the â€œSolvent-in-DESâ€•Regime upon the Replacement of Water by an Organic Solvent with Hydrogen Bond Capabilities. ACS Sustainable Chemistry and Engineering, 2020, 8, 12120-12131.	3.2	20

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19	Separation of CF₄/N₂, C₂F₆/N₂, and SF₆/N₂ Mixtures in Amorphous Activated Carbons Using Molecular Simulations. ACS Applied Materials & Interfaces, 2020, 12, 20044-20055.	4.0	19
20	Acetylene Storage and Separation Using Metalâ€“Organic Frameworks with Open Metal Sites. ACS Applied Materials & Interfaces, 2019, 11, 31499-31507.	4.0	43
21	Looking at the â€œWater-in-Deep-Eutectic-Solventâ€•System: A Dilution Range for High Performance Eutectics. ACS Sustainable Chemistry and Engineering, 2019, 7, 17565-17573.	3.2	80
22	Computational Study of the Effect of Functional Groups on Water Adsorption in Mesoporous Carbons: Implications for Gas Adsorption. ACS Applied Nano Materials, 2019, 2, 7103-7113.	2.4	21
23	Adsorption of Light Alcohols in a High Hydrophobic Metal Azolate Framework. Journal of Physical Chemistry C, 2019, 123, 23987-23994.	1.5	5
24	Enhancing the Water Capacity in Zr-Based Metalâ€“Organic Framework for Heat Pump and Atmospheric Water Generator Applications. ACS Applied Nano Materials, 2019, 2, 3050-3059.	2.4	18
25	Adsorption of Alkanes in Zeolites LTA and FAU: Quasi-Equilibrated Thermodesorption Supported by Molecular Simulations. Journal of Physical Chemistry C, 2019, 123, 29665-29678.	1.5	7
26	Adsorption and Diffusion of Benzene in Mg-MOF-74 with Open Metal Sites. ACS Applied Materials & Interfaces, 2019, 11, 4686-4700.	4.0	46
27	Improving Olefin Purification Using Metal Organic Frameworks with Open Metal Sites. ACS Applied Materials & Interfaces, 2018, 10, 16911-16917.	4.0	25
28	Phase Transition Induced by Gas Adsorption in Metalâ€Organic Frameworks. Chemistry - A European Journal, 2018, 24, 8530-8534.	1.7	15
29	Stepped Propane Adsorption in Pure-Silica ITW Zeolite. Langmuir, 2018, 34, 4774-4779.	1.6	10
30	Molecular Dynamics Analysis of Charge Transport in Ionicâ€Liquid Electrolytes Containing Added Salt with Mono, Di, and Trivalent Metal Cations. ChemPhysChem, 2018, 19, 1665-1673.	1.0	23
31	Potential of polarizable force fields for predicting the separation performance of small hydrocarbons in M-MOF-74. Physical Chemistry Chemical Physics, 2018, 20, 28848-28859.	1.3	18
32	Adsorption of Cyclohexane in Pure Silica Zeolites: Highâ€Throughput Computational Screening Validated by Experimental Data. ChemPhysChem, 2018, 19, 3364-3371.	1.0	8
33	Gate-Opening Mechanism of Hydrophilicâ€“Hydrophobic Metalâ€“Organic Frameworks: Molecular Simulations and Quasi-Equilibrated Desorption. Chemistry of Materials, 2018, 30, 5116-5127.	3.2	17
34	Role of Ionic Liquid [EMIM]⁺[SCN]^{â^'} in the Adsorption and Diffusion of Gases in Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2018, 10, 29694-29704.	4.0	38
35	Electrochemical Reduction of Oxygen in Aprotic Ionic Liquids Containing Metal Cations: A Case Study on the Naâ€“O₂ system. ChemSusChem, 2017, 10, 1616-1623.	3.6	30
36	Effective Model for Olefin/Paraffin Separation using (Co, Fe, Mn, Ni)â€MOFâ€74. ChemistrySelect, 2017, 2, 665-672.	0.7	16

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37	Ordering of n-Alkanes Adsorbed in the Micropores of AlPO₄-5: A Combined Molecular Simulations and Quasi-Equilibrated Thermodesorption Study. Journal of Physical Chemistry C, 2017, 121, 25292-25302.	1.5	16
38	Quasi-Equilibrated Thermodesorption Combined with Molecular Simulation for Adsorption and Separation of Hexane Isomers in Zeolites MFI and MEL. Journal of Physical Chemistry C, 2017, 121, 19226-19238.	1.5	11
39	Micelle Formation in Aqueous Solutions of Room Temperature Ionic Liquids: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2017, 121, 8348-8358.	1.2	39
40	Olefin/Paraffin Separation in Open Metal Site Cu-BTC Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2017, 121, 3126-3132.	1.5	37
41	Storage and Separation of Carbon Dioxide and Methane in Hydrated Covalent Organic Frameworks. Journal of Physical Chemistry C, 2016, 120, 23756-23762.	1.5	36
42	Adsorption of n-Alkanes in MFI and MEL: Quasi-Equilibrated Thermodesorption Combined with Molecular Simulations. Journal of Physical Chemistry C, 2016, 120, 25338-25350.	1.5	18
43	Aqueous Solutions of Ionic Liquids: Microscopic Assembly. ChemPhysChem, 2016, 17, 380-386.	1.0	14
44	Liquid self-diffusion of H₂O and DMF molecules in Co-MOF-74: molecular dynamics simulations and dielectric spectroscopy studies. Physical Chemistry Chemical Physics, 2016, 18, 19605-19612.	1.3	21
45	Quantum and Classical Molecular Dynamics of Ionic Liquid Electrolytes for Na/Liâ€based Batteries: Molecular Origins of the Conductivity Behavior. ChemPhysChem, 2016, 17, 2473-2481.	1.0	29
46	Computing bubble-points of CO2/CH4 gas mixtures in ionic liquids from Monte Carlo simulations. Fluid Phase Equilibria, 2016, 418, 100-107.	1.4	9
47	Solubilities of CO2, CH4, C2H6, and SO2 in ionic liquids and Selexol from Monte Carlo simulations. Journal of Computational Science, 2016, 15, 74-80.	1.5	31
48	Understanding and Exploiting Window Effects for Adsorption and Separations of Hydrocarbons. Journal of Physical Chemistry C, 2015, 119, 19236-19243.	1.5	13
49	Ion Transport in Electrolytes for Dye-Sensitized Solar Cells: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry C, 2014, 118, 28448-28455.	1.5	14
50	Solubility of the Precombustion Gases CO₂, CH₄, CO, H₂, N₂, and H₂S in the Ionic Liquid [bmim][Tf₂N] from Monte Carlo Simulations. Journal of Physical Chemistry C, 2014, 118, 23599-23604.	1.5	67
51	Molecular Mechanisms for Adsorption in Cu-BTC Metal Organic Framework. Journal of Physical Chemistry C, 2013, 117, 11357-11366.	1.5	81
52	Effect of Room-Temperature Ionic Liquids on CO₂ Separation by a Cu-BTC Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2013, 117, 20762-20768.	1.5	84