

Jose M Vicent-Luna

List of Publications by Year in descending order

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papers

1,261
citations

331259

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docs citations

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times ranked

1718
citing authors

#	ARTICLE	IF	CITATIONS
1	Effect of Room-Temperature Ionic Liquids on CO ₂ Separation by a Cu-BTC Metal-Organic Framework. <i>Journal of Physical Chemistry C</i> , 2013, 117, 20762-20768.	1.5	84
2	Molecular Mechanisms for Adsorption in Cu-BTC Metal Organic Framework. <i>Journal of Physical Chemistry C</i> , 2013, 117, 11357-11366.	1.5	81
3	Looking at the "Water-in-Deep-Eutectic-Solvent" System: A Dilution Range for High Performance Eutectics. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 17565-17573.	3.2	80
4	Solubility of the Precombustion Gases CO ₂ , CH ₄ , CO, H ₂ , N ₂ , and H ₂ S in the Ionic Liquid [bmim][Tf ₂ N] from Monte Carlo Simulations. <i>Journal of Physical Chemistry C</i> , 2014, 118, 23599-23604.	1.5	67
5	Adsorption and Diffusion of Benzene in Mg-MOF-74 with Open Metal Sites. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 4686-4700.	4.0	46
6	Acetylene Storage and Separation Using Metal-Organic Frameworks with Open Metal Sites. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 31499-31507.	4.0	43
7	Micelle Formation in Aqueous Solutions of Room Temperature Ionic Liquids: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2017, 121, 8348-8358.	1.2	39
8	Role of Ionic Liquid [EMIM] ⁺ [SCN] ⁻ in the Adsorption and Diffusion of Gases in Metal-Organic Frameworks. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 29694-29704.	4.0	38
9	Role of hydrogen bonding in the capture and storage of ammonia in zeolites. <i>Chemical Engineering Journal</i> , 2020, 387, 124062.	6.6	37
10	Olefin/Paraffin Separation in Open Metal Site Cu-BTC Metal-Organic Framework. <i>Journal of Physical Chemistry C</i> , 2017, 121, 3126-3132.	1.5	37
11	Storage and Separation of Carbon Dioxide and Methane in Hydrated Covalent Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2016, 120, 23756-23762.	1.5	36
12	Solubilities of CO ₂ , CH ₄ , C ₂ H ₆ , and SO ₂ in ionic liquids and Selexol from Monte Carlo simulations. <i>Journal of Computational Science</i> , 2016, 15, 74-80.	1.5	31
13	Atomistic Insights Into the Degradation of Inorganic Halide Perovskite CsPbI ₃ : A Reactive Force Field Molecular Dynamics Study. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 5519-5525.	2.1	31
14	Electrochemical Reduction of Oxygen in Aprotic Ionic Liquids Containing Metal Cations: A Case Study on the Na ⁺ O ₂ system. <i>ChemSusChem</i> , 2017, 10, 1616-1623.	3.6	30
15	Quantum and Classical Molecular Dynamics of Ionic Liquid Electrolytes for Na/Li-based Batteries: Molecular Origins of the Conductivity Behavior. <i>ChemPhysChem</i> , 2016, 17, 2473-2481.	1.0	29
16	π-Complexation for olefin/paraffin separation using aluminosilicates. <i>Chemical Engineering Journal</i> , 2020, 380, 122482.	6.6	28
17	Efficient modelling of ion structure and dynamics in inorganic metal halide perovskites. <i>Journal of Materials Chemistry A</i> , 2020, 8, 11824-11836.	5.2	26
18	Improving Olefin Purification Using Metal Organic Frameworks with Open Metal Sites. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 16911-16917.	4.0	25

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19	EMIMBF ₄ in ternary liquid mixtures of water, dimethyl sulfoxide and acetonitrile as tri-solvent-in-salt electrolytes for high-performance supercapacitors operating at -70 °C. <i>Energy Storage Materials</i> , 2021, 40, 368-385.	9.5	25
20	Effect of Co-Solvents on the Crystallization and Phase Distribution of Mixed-Dimensional Perovskites. <i>Advanced Energy Materials</i> , 2021, 11, 2102144.	10.2	25
21	Molecular Dynamics Analysis of Charge Transport in Ionic-Liquid Electrolytes Containing Added Salt with Mono, Di, and Trivalent Metal Cations. <i>ChemPhysChem</i> , 2018, 19, 1665-1673.	1.0	23
22	Exploiting the π -bonding for the separation of benzene and cyclohexane in zeolites. <i>Chemical Engineering Journal</i> , 2020, 398, 125678.	6.6	23
23	Transitioning from Ionic Liquids to Deep Eutectic Solvents. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 1232-1245.	3.2	22
24	Liquid self-diffusion of H ₂ O and DMF molecules in Co-MOF-74: molecular dynamics simulations and dielectric spectroscopy studies. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 19605-19612.	1.3	21
25	Computational Study of the Effect of Functional Groups on Water Adsorption in Mesoporous Carbons: Implications for Gas Adsorption. <i>ACS Applied Nano Materials</i> , 2019, 2, 7103-7113.	2.4	21
26	Further Extending the Dilution Range of the Solvent-in-DES Regime upon the Replacement of Water by an Organic Solvent with Hydrogen Bond Capabilities. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 12120-12131.	3.2	20
27	Separation of CF ₄ /N ₂ , C ₂ F ₆ /N ₂ , and SF ₆ /N ₂ Mixtures in Amorphous Activated Carbons Using Molecular Simulations. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 20044-20055.	4.0	19
28	Adsorption of <i>n</i> -Alkanes in MFI and MEL: Quasi-Equilibrated Thermodesorption Combined with Molecular Simulations. <i>Journal of Physical Chemistry C</i> , 2016, 120, 25338-25350.	1.5	18
29	Potential of polarizable force fields for predicting the separation performance of small hydrocarbons in M-MOF-74. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 28848-28859.	1.3	18
30	Enhancing the Water Capacity in Zr-Based Metal-Organic Framework for Heat Pump and Atmospheric Water Generator Applications. <i>ACS Applied Nano Materials</i> , 2019, 2, 3050-3059.	2.4	18
31	Gate-Opening Mechanism of Hydrophilic-Hydrophobic Metal-Organic Frameworks: Molecular Simulations and Quasi-Equilibrated Desorption. <i>Chemistry of Materials</i> , 2018, 30, 5116-5127.	3.2	17
32	Effective Model for Olefin/Paraffin Separation using (Co, Fe, Mn, Ni)-MOF-74. <i>ChemistrySelect</i> , 2017, 2, 665-672.	0.7	16
33	Ordering of <i>n</i> -Alkanes Adsorbed in the Micropores of AlPO ₄ -5: A Combined Molecular Simulations and Quasi-Equilibrated Thermodesorption Study. <i>Journal of Physical Chemistry C</i> , 2017, 121, 25292-25302.	1.5	16
34	Efficient Computation of Structural and Electronic Properties of Halide Perovskites Using Density Functional Tight Binding: GFN1-xTB Method. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4415-4424.	2.5	16
35	Phase Transition Induced by Gas Adsorption in Metal-Organic Frameworks. <i>Chemistry - A European Journal</i> , 2018, 24, 8530-8534.	1.7	15
36	Ion Transport in Electrolytes for Dye-Sensitized Solar Cells: A Combined Experimental and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2014, 118, 28448-28455.	1.5	14

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37	Aqueous Solutions of Ionic Liquids: Microscopic Assembly. ChemPhysChem, 2016, 17, 380-386.	1.0	14
38	Understanding and Exploiting Window Effects for Adsorption and Separations of Hydrocarbons. Journal of Physical Chemistry C, 2015, 119, 19236-19243.	1.5	13
39	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
40	Stepped Propane Adsorption in Pure-Silica ITW Zeolite. Langmuir, 2018, 34, 4774-4779.	1.6	10
41	Enhancing separation efficiency in European syngas industry by using zeolites. Catalysis Today, 2021, 362, 113-121.	2.2	10
42	Water-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
43	Computing bubble-points of CO ₂ /CH ₄ gas mixtures in ionic liquids from Monte Carlo simulations. Fluid Phase Equilibria, 2016, 418, 100-107.	1.4	9
44	Phase transformation barrier modulation of CsPbI ₃ films via PbI ₃ ²⁻ complex for efficient all-inorganic perovskite photovoltaics. Nano Energy, 2022, 99, 107388.	8.2	9
45	Adsorption of Cyclohexane in Pure Silica Zeolites: High-Throughput Computational Screening Validated by Experimental Data. ChemPhysChem, 2018, 19, 3364-3371.	1.0	8
46	Aqueous Co-solvent in Zwitterionic-based Protic Ionic Liquids as Electrolytes in 2.0 V Supercapacitors. ChemSusChem, 2020, 13, 5983-5995.	3.6	8
47	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
48	Adsorption of Light Alcohols in a High Hydrophobic Metal Azolate Framework. Journal of Physical Chemistry C, 2019, 123, 23987-23994.	1.5	5
49	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
50	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
51	Refined GFN1-xTB Parameters for Engineering Phase-Stable CsPbX ₃ Perovskites. Journal of Physical Chemistry C, 2022, 126, 9587-9596.	1.5	2
52	Effect of Co-solvents on the Crystallization and Phase Distribution of Mixed-Dimensional Perovskites (Adv. Energy Mater. 42/2021). Advanced Energy Materials, 2021, 11, 2170168.	10.2	0