# David S Sholl

## List of Publications by Year in Descending Order



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| 240 papers | 16,759 citations | 70 h-index | 122 g-index |
| 249 ext. papers | 19,279 ext. citations | 7.2 avg, IF | 7.47 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 240 | Exemplar Mixtures for Studying Complex Mixture Effects in Practical Chemical Separations.. *Jacs Au* , **2022**, 2, 322-327 | | 5 |
| 239 | Single-walled zeolitic nanotubes.. *Science*, **2022**, 375, 62-66 | 33.3 | 5 |
| 238 | In silico design of microporous polymers for chemical separations and storage. *Current Opinion in Chemical Engineering*, **2022**, 36, 100795 | 5.4 | 1 |
| 237 | Comprehensive Assessment of the Accuracy of the Ideal Adsorbed Solution Theory for Predicting Binary Adsorption of Gas Mixtures in Porous Materials. *Industrial & Engineering Chemistry Research*, **2022**, 61, 727-739 | 3.9 | 3 |
| 236 | Discrepancy quantification between experimental and simulated data of CO2 adsorption isotherm using hierarchical Bayesian estimation. *Separation and Purification Technology*, **2022**, 121371 | 8.3 | 0 |
| 235 | A Collection of More than 900 Gas Mixture Adsorption Experiments in Porous Materials from Literature Meta-Analysis. *Industrial & Engineering Chemistry Research*, **2021**, 60, 639-651 | 3.9 | 22 |
| 234 | Quantifying Impact of Intrinsic Flexibility on Molecular Adsorption in Zeolites. *Journal of Physical Chemistry C*, **2021**, 125, 5296-5305 | 3.8 | 4 |
| 233 | Construction of an Anion-Pillared MOF Database and the Screening of MOFs Suitable for Xe/Kr Separation. *ACS Applied Materials & Interfaces*, **2021**, 13, 11039-11049 | 9.5 | 18 |
| 232 | A Transferable Force Field for Predicting Adsorption and Diffusion of Hydrocarbons and Small Molecules in Silica Zeolites with Coupled-Cluster Accuracy. *Journal of Physical Chemistry C*, **2021**, 125, 8418-8429 | 3.8 | 4 |
| 231 | Adsorption space for microporous polymers with diverse adsorbate species. *Npj Computational Materials*, **2021**, 7, | 10.9 | 6 |
| 230 | Interpretable Machine Learning-Based Predictions of Methane Uptake Isotherms in Metal□Organic Frameworks. *Chemistry of Materials*, **2021**, 33, 3543-3552 | 9.6 | 12 |
| 229 | In-situ IR Spectroscopy Study of Reactions of C3 Oxygenates on Heteroatom (Sn, Mo, and W) doped BEA Zeolites and the Effect of Co-adsorbed Water. *ChemCatChem*, **2021**, 13, 445-458 | 5.2 | 2 |
| 228 | Adsorption-Based Separation of Near-Azeotropic Mixtures-A Challenging Example for High-Throughput Development of Adsorbents. *Journal of Physical Chemistry B*, **2021**, 125, 926-936 | 3.4 | 5 |
| 227 | Fingerprinting diverse nanoporous materials for optimal hydrogen storage conditions using meta-learning. *Science Advances*, **2021**, 7, | 14.3 | 8 |
| 226 | Efficient Models for Predicting Temperature-Dependent Henry□s Constants and Adsorption Selectivities for Diverse Collections of Molecules in Metal□Organic Frameworks. *Journal of Physical Chemistry C*, **2021**, 125, 18046-18057 | 3.8 | 6 |
| 225 | High-Throughput Screening of Anion-Pillared Metal□Organic Frameworks for the Separation of Light Hydrocarbons. *Journal of Physical Chemistry C*, **2021**, 125, 20076-20086 | 3.8 | 4 |
| 224 | Analysis of energetics and economics of sub-ambient hybrid post-combustion carbon dioxide capture. *AICHE Journal*, **2021**, 67, e17403 | 3.6 | 3 |

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| 223 | Incorporating Flexibility Effects into Metal-Organic Framework Adsorption Simulations Using Different Models.. *ACS Applied Materials & Interfaces*, **2021**, 13, 61305-61315 | 9.5 | 2 |
| 222 | Spin-Crossover Effects in Reversible O2 Binding on a Dinuclear Cobalt(II) Complex. *Journal of Physical Chemistry C*, **2020**, 124, 26843-26850 | 3.8 | 1 |
| 221 | Using Site Heterogeneity in Metal□Organic Frameworks with Bimetallic Open Metal Sites for Olefin/Paraffin Separations. *ACS Applied Nano Materials*, **2020**, 3, 5291-5300 | 5.6 | 4 |
| 220 | Molecular Dynamics Investigation of Surface Resistances in Zeolite Nanosheets. *Journal of Physical Chemistry C*, **2020**, 124, 15241-15252 | 3.8 | 10 |
| 219 | Tuning the Wettability of Metal-Organic Frameworks via Defect Engineering for Efficient Oil/Water Separation. *ACS Applied Materials & Interfaces*, **2020**, 12, 34413-34422 | 9.5 | 15 |
| 218 | Effect of Humidity on the Sorption of H2S from Multicomponent Acid Gas Streams on Silica-Supported Sterically Hindered and Unhindered Amines. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 10102-10114 | 8.3 | 11 |
| 217 | Selecting Adsorbents to Separate Diverse Near-Azeotropic Chemicals. *Journal of Physical Chemistry C*, **2020**, 124, 3664-3670 | 3.8 | 22 |
| 216 | Impact of intrinsic framework flexibility for selective adsorption of sarin in non-aqueous solvents using metal-organic frameworks. *Physical Chemistry Chemical Physics*, **2020**, 22, 6441-6448 | 3.6 | 18 |
| 215 | How Well Do Approximate Models of Adsorption-Based CO2 Capture Processes Predict Results of Detailed Process Models?. *Industrial & Engineering Chemistry Research*, **2020**, 59, 7097-7108 | 3.9 | 35 |
| 214 | Does repeat synthesis in materials chemistry obey a power law?. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 877-882 | 11.5 | 23 |
| 213 | Understanding Dealumination Mechanisms in Protonic and Cationic Zeolites. *Journal of Physical Chemistry C*, **2020**, 124, 668-676 | 3.8 | 13 |
| 212 | Quantitative Correlations for the Durability of Zeolitic Imidazolate Frameworks in Humid SO2. *Industrial & Engineering Chemistry Research*, **2020**, 59, 245-252 | 3.9 | 4 |
| 211 | A Strong Test of Atomically Detailed Models of Molecular Adsorption in Zeolites Using Multilaboratory Experimental Data for CO Adsorption in Ammonium ZSM-5. *Journal of Physical Chemistry Letters*, **2020**, 11, 471-477 | 6.4 | 16 |
| 210 | Hierarchical Bayesian estimation for adsorption isotherm parameter determination. *Chemical Engineering Science*, **2020**, 214, 115435 | 4.4 | 11 |
| 209 | Experimentally Verified Alcohol Adsorption Isotherms in Nanoporous Materials from Literature Meta-Analysis. *Journal of Chemical & Engineering Data*, **2020**, 65, 4970-4979 | 2.8 | 12 |
| 208 | A Database of Porous Rigid Amorphous Materials. *Chemistry of Materials*, **2020**, 32, 8020-8033 | 9.6 | 16 |
| 207 | Quantitatively Predicting Impact of Structural Flexibility on Molecular Diffusion in Small Pore Metal□Organic Frameworks□A Molecular Dynamics Study of Hypothetical ZIF-8 Polymorphs. *Journal of Physical Chemistry C*, **2020**, 124, 20203-20212 | 3.8 | 5 |
| 206 | Tuning the Structures of Metal□Organic Frameworks via a Mixed-Linker Strategy for Ethylene/Ethane Kinetic Separation. *Chemistry of Materials*, **2020**, 32, 3715-3722 | 9.6 | 19 |

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| 205 | Synthesizing New Hybrid Zeolitic Imidazolate Frameworks by Controlled Demolition and Reconstruction **2019**, 1, 447-451 | | 4 |
| 204 | Five Easy Ways To Make Your Research More Reproducible. *Langmuir*, **2019**, 35, 13257-13258 | 4 | 4 |
| 203 | Predictions of Hg0 and HgCl2 Adsorption Properties in UiO-66 from Flue Gas Using Molecular Simulations. *Journal of Physical Chemistry C*, **2019**, 123, 5972-5979 | 3.8 | 13 |
| 202 | Sorption and Transport of Vapors in ZIF-11: Adsorption, Diffusion, and Linker Flexibility. *Journal of Physical Chemistry C*, **2019**, | 3.8 | 11 |
| 201 | Screening Diffusion of Small Molecules in Flexible Zeolitic Imidazolate Frameworks Using a DFT-Parameterized Force Field. *Journal of Physical Chemistry C*, **2019**, 123, 9153-9167 | 3.8 | 19 |
| 200 | Does Chemical Engineering Research Have a Reproducibility Problem?. *Annual Review of Chemical and Biomolecular Engineering*, **2019**, 10, 43-57 | 8.9 | 14 |
| 199 | Propagation of Degradation-Induced Defects in Zeolitic Imidazolate Frameworks. *Journal of Physical Chemistry C*, **2019**, 123, 6655-6666 | 3.8 | 11 |
| 198 | Significant Temperature Dependence of the Isosteric Heats of Adsorption of Gases in Zeolites Demonstrated by Experiments and Molecular Simulations. *Journal of Physical Chemistry C*, **2019**, 123, 20405-20412 | 3.8 | 16 |
| 197 | Effects of Intrinsic Flexibility on Adsorption Properties of Metal-Organic Frameworks at Dilute and Nondilute Loadings. *ACS Applied Materials & Interfaces*, **2019**, 11, 31060-31068 | 9.5 | 39 |
| 196 | Rapid Prediction of Adsorption Isotherms of a Diverse Range of Molecules in Hyper-Cross-Linked Polymers. *Journal of Physical Chemistry C*, **2019**, 123, 17884-17893 | 3.8 | 10 |
| 195 | Advances, Updates, and Analytics for the Computation-Ready, Experimental Metal□Organic Framework Database: CoRE MOF 2019. *Journal of Chemical & Engineering Data*, **2019**, 64, 5985-5998 | 2.8 | 183 |
| 194 | Determining Diffusion Coefficients of Chemical Warfare Agents in Metal-Organic Frameworks. *Journal of Physical Chemistry Letters*, **2019**, 10, 7823-7830 | 6.4 | 19 |
| 193 | In Silico Prediction of Structural Properties of a Racemic Porous Organic Cage Crystal. *Journal of Physical Chemistry C*, **2019**, 123, 1720-1729 | 3.8 | 5 |
| 192 | Stability of Zeolitic Imidazolate Frameworks in NO2. *Journal of Physical Chemistry C*, **2019**, 123, 2336-2346 | 3.8 | 22 |
| 191 | Moving Beyond Adsorption Capacity in Design of Adsorbents for CO2 Capture from Ultradilute Feeds: Kinetics of CO2 Adsorption in Materials with Stepped Isotherms. *Industrial & Engineering Chemistry Research*, **2019**, 58, 366-377 | 3.9 | 30 |
| 190 | Database of Computation-Ready 2D Zeolitic Slabs. *Chemistry of Materials*, **2019**, 31, 353-364 | 9.6 | 12 |
| 189 | Quantitative Predictions of Molecular Diffusion in Binary Mixed-Linker Zeolitic Imidazolate Frameworks Using Molecular Simulations. *Journal of Physical Chemistry C*, **2018**, 122, 5627-5638 | 3.8 | 10 |
| 188 | Competitive Binding of Ethylene, Water, and Carbon Monoxide in Metal□Organic Framework Materials with Open Cu Sites. *Journal of Physical Chemistry C*, **2018**, 122, 8960-8966 | 3.8 | 24 |

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| 187 | Efficiently Exploring Adsorption Space to Identify Privileged Adsorbents for Chemical Separations of a Diverse Set of Molecules. *ChemSusChem*, **2018**, 11, 1567-1575 | 8.3 | 39 |
| 186 | Insights into the Stability of Zeolitic Imidazolate Frameworks in Humid Acidic Environments from First-Principles Calculations. *Journal of Physical Chemistry C*, **2018**, 122, 4339-4348 | 3.8 | 37 |
| 185 | Liquid-Phase Multicomponent Adsorption and Separation of Xylene Mixtures by Flexible MIL-53 Adsorbents. *Journal of Physical Chemistry C*, **2018**, 122, 386-397 | 3.8 | 36 |
| 184 | Writing Theory and Modeling Papers for Langmuir: The Good, the Bad, and the Ugly. *Langmuir*, **2018**, 34, 1817-1818 | 4 | 2 |
| 183 | Molecular Simulation of Capture of Sulfur-Containing Gases by Porous Aromatic Frameworks. *Journal of Physical Chemistry C*, **2018**, 122, 18456-18467 | 3.8 | 15 |
| 182 | Formation Mechanisms and Defect Engineering of Imine-Based Porous Organic Cages. *Chemistry of Materials*, **2018**, 30, 262-272 | 9.6 | 34 |
| 181 | Tuning Binding Tendencies of Small Molecules in Metal□Organic Frameworks with Open Metal Sites by Metal Substitution and Linker Functionalization. *Journal of Physical Chemistry C*, **2018**, 122, 27486-27494 | 3.8 | 23 |
| 180 | How Useful Are Common Simulants of Chemical Warfare Agents at Predicting Adsorption Behavior?. *Journal of Physical Chemistry C*, **2018**, 122, 26061-26069 | 3.8 | 37 |
| 179 | Acid Gas Stability of Zeolitic Imidazolate Frameworks: Generalized Kinetic and Thermodynamic Characteristics. *Chemistry of Materials*, **2018**, 30, 4089-4101 | 9.6 | 49 |
| 178 | The Effect of Aluminum Short-Range Ordering on Carbon Dioxide Adsorption in Zeolites. *Journal of Physical Chemistry C*, **2018**, 122, 12332-12340 | 3.8 | 16 |
| 177 | First-Principles-Derived Force Fields for CH4 Adsorption and Diffusion in Siliceous Zeolites. *Journal of Physical Chemistry C*, **2018**, 122, 12880-12891 | 3.8 | 17 |
| 176 | Assessing the Impact of Point Defects on Molecular Diffusion in ZIF-8 Using Molecular Simulations. *Journal of Physical Chemistry Letters*, **2018**, 9, 4037-4044 | 6.4 | 25 |
| 175 | From water to organics in membrane separations. *Nature Materials*, **2017**, 16, 276-279 | 27 | 235 |
| 174 | Acid Gas Adsorption on Metal-Organic Framework Nanosheets as a Model of an "All-Surface" Material. *Journal of Chemical Theory and Computation*, **2017**, 13, 1341-1350 | 6.4 | 20 |
| 173 | Modeling and process simulation of hollow fiber membrane reactor systems for propane dehydrogenation. *AICHE Journal*, **2017**, 63, 4519-4531 | 3.6 | 12 |
| 172 | Monolith-Supported Amine-Functionalized Mg(dobpdc) Adsorbents for CO Capture. *ACS Applied Materials & Interfaces*, **2017**, 9, 17042-17050 | 9.5 | 53 |
| 171 | Understanding Structure, Metal Distribution, and Water Adsorption in Mixed-Metal MOF-74. *Journal of Physical Chemistry C*, **2017**, 121, 627-635 | 3.8 | 37 |
| 170 | Establishing upper bounds on CO2 swing capacity in sub-ambient pressure swing adsorption via molecular simulation of metal□organic frameworks. *Journal of Materials Chemistry A*, **2017**, 5, 12258-12265 | 13 | 38 |

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| 169 | Lattice-Gas Modeling of Adsorbate Diffusion in Mixed-Linker Zeolitic Imidazolate Frameworks: Effect of Local Imidazolate Ordering. *Langmuir*, **2017**, 33, 6481-6491 | 4 | 8 |
| 168 | Temperature-regulated guest admission and release in microporous materials. *Nature Communications*, **2017**, 8, 15777 | 17.4 | 36 |
| 167 | First-principles investigation of chemical stability and proton conductivity of M-doped BaZrO3 (M=K, Rb, and Cs). *Journal of the American Ceramic Society*, **2017**, 100, 2997-3003 | 3.8 | 9 |
| 166 | Structural and Mechanistic Differences in Mixed-Linker Zeolitic Imidazolate Framework Synthesis by Solvent Assisted Linker Exchange and de Novo Routes. *Journal of the American Chemical Society*, **2017**, 139, 5906-5915 | 16.4 | 81 |
| 165 | Propane dehydrogenation catalyzed by gallosilicate MFI zeolites with perturbed acidity. *Journal of Catalysis*, **2017**, 345, 113-123 | 7.3 | 86 |
| 164 | Research Challenges in Avoiding Showstoppers in Developing Materials for Large-Scale Energy Applications. *Joule*, **2017**, 1, 208-211 | 27.8 | 28 |
| 163 | Recovery of Acid-Gas-Degraded Zeolitic Imidazolate Frameworks by Solvent-Assisted Crystal Redemption (SACRed). *ACS Applied Materials & Interfaces*, **2017**, 9, 34597-34602 | 9.5 | 15 |
| 162 | Effect of Surface Structure of TiO2 Nanoparticles on CO2 Adsorption and SO2 Resistance. *ACS Sustainable Chemistry and Engineering*, **2017**, 5, 9295-9306 | 8.3 | 29 |
| 161 | Heat-Treatment of Defective UiO-66 from Modulated Synthesis: Adsorption and Stability Studies. *Journal of Physical Chemistry C*, **2017**, 121, 23471-23479 | 3.8 | 42 |
| 160 | CO2 Dynamics in Pure and Mixed-Metal MOFs with Open Metal Sites. *Journal of Physical Chemistry C*, **2017**, 121, 25778-25787 | 3.8 | 49 |
| 159 | Butanol Separation from Humid CO2-Containing Multicomponent Vapor Mixtures by Zeolitic Imidazolate Frameworks. *ACS Sustainable Chemistry and Engineering*, **2017**, 5, 9467-9476 | 8.3 | 30 |
| 158 | Computational Screening of Functionalized UiO-66 Materials for Selective Contaminant Removal from Air. *Journal of Physical Chemistry C*, **2017**, 121, 20396-20406 | 3.8 | 22 |
| 157 | Hierarchical Ga-MFI Catalysts for Propane Dehydrogenation. *Chemistry of Materials*, **2017**, 29, 7213-7222 | 9.6 | 58 |
| 156 | How Reproducible Are Isotherm Measurements in Metal–Organic Frameworks?. *Chemistry of Materials*, **2017**, 29, 10487-10495 | 9.6 | 98 |
| 155 | Impacts of Gas Impurities from Pipeline Natural Gas on Methane Storage in Metal–Organic Frameworks during Long-Term Cycling. *Journal of Physical Chemistry C*, **2017**, 121, 15735-15745 | 3.8 | 22 |
| 154 | Computational investigation on CO2 adsorption in titanium carbide-derived carbons with residual titanium. *Carbon*, **2017**, 111, 741-751 | 10.4 | 9 |
| 153 | Large-Scale Refinement of Metal–Organic Framework Structures Using Density Functional Theory. *Chemistry of Materials*, **2017**, 29, 2521-2528 | 9.6 | 74 |
| 152 | One-Step Synthesis of Zeolite Membranes Containing Catalytic Metal Nanoclusters. *ACS Applied Materials & Interfaces*, **2016**, 8, 24671-81 | 9.5 | 20 |

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| 151 | Interactions of SO2-Containing Acid Gases with ZIF-8: Structural Changes and Mechanistic Investigations. *Journal of Physical Chemistry C*, **2016**, 120, 27221-27229 | 3.8 | 71 |
| 150 | Direct Air Capture of CO2 Using Amine Functionalized MIL-101(Cr). *ACS Sustainable Chemistry and Engineering*, **2016**, 4, 5761-5768 | 8.3 | 131 |
| 149 | Propane Dehydrogenation over Alumina-Supported Iron/Phosphorus Catalysts: Structural Evolution of Iron Species Leading to High Activity and Propylene Selectivity. *ACS Catalysis*, **2016**, 6, 5673-5683 | 13.1 | 79 |
| 148 | Seven chemical separations to change the world. *Nature*, **2016**, 532, 435-7 | 50.4 | 1625 |
| 147 | Thin Hydrogen-Selective SAPO-34 Zeolite Membranes for Enhanced Conversion and Selectivity in Propane Dehydrogenation Membrane Reactors. *Chemistry of Materials*, **2016**, 28, 4397-4402 | 9.6 | 41 |
| 146 | Improved HillSauer Force Field for Accurate Description of Pores in 8-Ring Zeolites. *Journal of Physical Chemistry C*, **2016**, 120, 14140-14148 | 3.8 | 14 |
| 145 | A Comprehensive Set of High-Quality Point Charges for Simulations of MetalOrganic Frameworks. *Chemistry of Materials*, **2016**, 28, 785-793 | 9.6 | 95 |
| 144 | Computational Characterization of Defects in Metal-Organic Frameworks: Spontaneous and Water-Induced Point Defects in ZIF-8. *Journal of Physical Chemistry Letters*, **2016**, 7, 459-64 | 6.4 | 82 |
| 143 | Effect of Framework Flexibility on C8 Aromatic Adsorption at High Loadings in MetalOrganic Frameworks. *Journal of Physical Chemistry C*, **2016**, 120, 370-376 | 3.8 | 35 |
| 142 | Transition State Theory Methods To Measure Diffusion in Flexible Nanoporous Materials: Application to a Porous Organic Cage Crystal. *Journal of Physical Chemistry C*, **2016**, 120, 1110-1120 | 3.8 | 40 |
| 141 | Engineering Porous Organic Cage Crystals with Increased Acid Gas Resistance. *Chemistry - A European Journal*, **2016**, 22, 10743-7 | 4.8 | 24 |
| 140 | Computational Model and Characterization of Stacking Faults in ZIF-8 Polymorphs. *Journal of Physical Chemistry C*, **2016**, 120, 27380-27388 | 3.8 | 12 |
| 139 | Synergistic Effects of Water and SO2 on Degradation of MIL-125 in the Presence of Acid Gases. *Journal of Physical Chemistry C*, **2016**, 120, 27230-27240 | 3.8 | 59 |
| 138 | Propane Dehydrogenation over In2O3Ga2O3Al2O3 Mixed Oxides. *ChemCatChem*, **2016**, 8, 214-221 | 5.2 | 41 |
| 137 | Computational Identification and Experimental Evaluation of MetalOrganic Frameworks for Xylene Enrichment. *Journal of Physical Chemistry C*, **2016**, 120, 12075-12082 | 3.8 | 37 |
| 136 | Identification of High-CO2-Capacity Cationic Zeolites by Accurate Computational Screening. *Chemistry of Materials*, **2016**, 28, 3887-3896 | 9.6 | 46 |
| 135 | Structure Elucidation of Mixed-Linker Zeolitic Imidazolate Frameworks by Solid-State (1)H CRAMPS NMR Spectroscopy and Computational Modeling. *Journal of the American Chemical Society*, **2016**, 138, 7325-36 | 16.4 | 39 |
| 134 | CO2 capture via adsorption in amine-functionalized sorbents. *Current Opinion in Chemical Engineering*, **2016**, 12, 82-90 | 5.4 | 84 |

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| 133 | Effects of Open Metal Site Availability on Adsorption Capacity and Olefin/Paraffin Selectivity in the Metal□Organic Framework Cu3(BTC)2. *Industrial & Engineering Chemistry Research*, **2016**, 55, 5043-5053 | 3.9 | 16 |
| 132 | Facet-Specific Stability of ZIF-8 in the Presence of Acid Gases Dissolved in Aqueous Solutions. *Chemistry of Materials*, **2016**, 28, 6960-6967 | 9.6 | 96 |
| 131 | Screening of Copper Open Metal Site MOFs for Olefin/Paraffin Separations Using DFT-Derived Force Fields. *Journal of Physical Chemistry C*, **2016**, 120, 23044-23054 | 3.8 | 45 |
| 130 | DFT-Derived Force Fields for Modeling Hydrocarbon Adsorption in MIL-47(V). *Langmuir*, **2015**, 31, 8453-68 | 4 | 27 |
| 129 | Efficient Calculation of Gas Diffusivity in Single-Component and Binary Mixtures of Spherical Adsorbates in Flexible 8MR Zeolites. *Journal of Physical Chemistry C*, **2015**, 119, 16596-16605 | 3.8 | 13 |
| 128 | Prediction of Adsorption Properties of Cyclic Hydrocarbons in MOFs Using DFT-Derived Force Fields. *Journal of Physical Chemistry C*, **2015**, 119, 16920-16926 | 3.8 | 16 |
| 127 | Modeling Diffusion of Linear Hydrocarbons in Silica Zeolite LTA Using Transition Path Sampling. *Journal of Physical Chemistry C*, **2015**, 119, 15643-15653 | 3.8 | 19 |
| 126 | Fluorinated carbide-derived carbon: more hydrophilic, yet apparently more hydrophobic. *Journal of the American Chemical Society*, **2015**, 137, 5969-79 | 16.4 | 17 |
| 125 | Highly tunable molecular sieving and adsorption properties of mixed-linker zeolitic imidazolate frameworks. *Journal of the American Chemical Society*, **2015**, 137, 4191-7 | 16.4 | 155 |
| 124 | Computational Prediction of Metal Organic Frameworks Suitable for Molecular Infiltration as a Route to Development of Conductive Materials. *Journal of Physical Chemistry Letters*, **2015**, 6, 1586-91 | 6.4 | 35 |
| 123 | Defects in Metal-Organic Frameworks: Challenge or Opportunity?. *Journal of Physical Chemistry Letters*, **2015**, 6, 3437-44 | 6.4 | 230 |
| 122 | DFT-based force field development for noble gas adsorption in metal organic frameworks. *Journal of Materials Chemistry A*, **2015**, 3, 23539-23548 | 13 | 24 |
| 121 | Benchmarking density functional theory predictions of framework structures and properties in a chemically diverse test set of metal□organic frameworks. *Journal of Materials Chemistry A*, **2015**, 3, 22432-22440 | 13 | 49 |
| 120 | Large-Scale Computational Screening of Binary Intermetallics for Membrane-Based Hydrogen Separation. *Journal of Physical Chemistry C*, **2015**, 119, 26319-26326 | 3.8 | 7 |
| 119 | Predicting multicomponent adsorption: 50 years of the ideal adsorbed solution theory. *AICHE Journal*, **2015**, 61, 2757-2762 | 3.6 | 219 |
| 118 | Impact of branching on the supramolecular assembly of thioethers on Au(111). *Journal of Chemical Physics*, **2015**, 142, 101915 | 3.9 | 9 |
| 117 | Temperature and Loading-Dependent Diffusion of Light Hydrocarbons in ZIF-8 as Predicted Through Fully Flexible Molecular Simulations. *Journal of the American Chemical Society*, **2015**, 137, 15760-71 | 16.4 | 121 |
| 116 | High-Tc Layered Ferrielectric Crystals by Coherent Spinodal Decomposition. *ACS Nano*, **2015**, 9, 12365-73 | 16.7 | 39 |

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| 115 | Material properties and operating configurations of membrane reactors for propane dehydrogenation. *AICHE Journal*, **2015**, 61, 922-935 | 3.6 | 16 |
| 114 | The materials genome in action: identifying the performance limits for methane storage. *Energy and Environmental Science*, **2015**, 8, 1190-1199 | 35.4 | 263 |
| 113 | Investigation of the adsorption of amino acids on Pd(111): A density functional theory study. *Applied Surface Science*, **2014**, 301, 199-207 | 6.7 | 12 |
| 112 | Recent developments in first-principles force fields for molecules in nanoporous materials. *Journal of Materials Chemistry A*, **2014**, 2, 274-291 | 13 | 104 |
| 111 | Computation-Ready, Experimental Metal□Organic Frameworks: A Tool To Enable High-Throughput Screening of Nanoporous Crystals. *Chemistry of Materials*, **2014**, 26, 6185-6192 | 9.6 | 387 |
| 110 | Thermal, Oxidative and CO2 Induced Degradation of Primary Amines Used for CO2 Capture: Effect of Alkyl Linker on Stability. *Journal of Physical Chemistry C*, **2014**, 118, 12302-12311 | 3.8 | 80 |
| 109 | Role of Lewis and Br□sted Acid Sites in the Dehydration of Glycerol over Niobia. *ACS Catalysis*, **2014**, 4, 3180-3192 | 13.1 | 124 |
| 108 | Adsorption and Diffusion of 4d and 5d Transition Metal Adatoms on Graphene/Ru(0001) and the Implications for Cluster Nucleation. *Topics in Catalysis*, **2014**, 57, 69-79 | 2.3 | 22 |
| 107 | Control of Metal□Organic Framework Crystal Topology by Ligand Functionalization: Functionalized HKUST-1 Derivatives. *Crystal Growth and Design*, **2014**, 14, 6122-6128 | 3.5 | 43 |
| 106 | Crystal-Size-Dependent Structural Transitions in Nanoporous Crystals: Adsorption-Induced Transitions in ZIF-8. *Journal of Physical Chemistry C*, **2014**, 118, 20727-20733 | 3.8 | 118 |
| 105 | Powered by DFT: Screening methods that accelerate materials development for hydrogen in metals applications. *Accounts of Chemical Research*, **2014**, 47, 3275-83 | 24.3 | 13 |
| 104 | Molecular dynamics simulation of framework flexibility effects on noble gas diffusion in HKUST-1 and ZIF-8. *Microporous and Mesoporous Materials*, **2014**, 194, 190-199 | 5.3 | 61 |
| 103 | First principles studies of proton conduction in KTaO3. *Journal of Chemical Physics*, **2014**, 141, 024707 | 3.9 | 6 |
| 102 | Near Surface Phase Transition of Solute Derived Pt Monolayers. *Topics in Catalysis*, **2013**, 56, 1065-1073 | 2.3 | 8 |
| 101 | Characterization of the Thermodynamic Stability of Solvated Metal□Organic Framework Polymorphs Using Molecular Simulations. *Journal of Physical Chemistry C*, **2013**, 117, 20636-20642 | 3.8 | 25 |
| 100 | Exploring the Framework Hydrophobicity and Flexibility of ZIF-8: From Biofuel Recovery to Hydrocarbon Separations. *Journal of Physical Chemistry Letters*, **2013**, 4, 3618-3622 | 6.4 | 242 |
| 99 | First principles derived, transferable force fields for CO2 adsorption in Na-exchanged cationic zeolites. *Physical Chemistry Chemical Physics*, **2013**, 15, 12882-94 | 3.6 | 58 |
| 98 | Rapid prediction of hydrogen permeation through amorphous metal membranes: an efficient computational screening approach. *Energy and Environmental Science*, **2013**, 6, 232-240 | 35.4 | 18 |

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| 97 | Adsorption and Diffusion of Small Alcohols in Zeolitic Imidazolate Frameworks ZIF-8 and ZIF-90. *Journal of Physical Chemistry C*, **2013**, 117, 3169-3176 | 3.8 | 111 |
| 96 | MOF stability and gas adsorption as a function of exposure to water, humid air, SO2, and NO2. *Microporous and Mesoporous Materials*, **2013**, 173, 86-91 | 5.3 | 81 |
| 95 | Prediction of Water Adsorption in Copper-Based Metal□Organic Frameworks Using Force Fields Derived from Dispersion-Corrected DFT Calculations. *Journal of Physical Chemistry C*, **2013**, 117, 7519-7525 | 3.8 | 46 |
| 94 | First principles assessment of perovskite dopants for proton conductors with chemical stability and high conductivity. *RSC Advances*, **2013**, 3, 3333 | 3.7 | 20 |
| 93 | Efficient and Accurate Methods for Characterizing Effects of Framework Flexibility on Molecular Diffusion in Zeolites: CH4 Diffusion in Eight Member Ring Zeolites. *Journal of Physical Chemistry C*, **2013**, 117, 13462-13473 | 3.8 | 45 |
| 92 | First-Principles Models of Facilitating H2 Transport through Metal Films Using Spillover. *Journal of Physical Chemistry C*, **2013**, 117, 1217-1223 | 3.8 | 10 |
| 91 | Surface interactions of C and C(3) polyols with □Al2O3 and the role of coadsorbed water. *Langmuir*, **2013**, 29, 581-93 | 4 | 58 |
| 90 | Ultem□ /ZIF-8 mixed matrix hollow fiber membranes for CO2/N2 separations. *Journal of Membrane Science*, **2012**, 401-402, 76-82 | 9.6 | 253 |
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