

# Gustavo A Orozco

## List of Publications by Year in descending order

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11  
papers

245  
citations

1307594

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h-index

1281871

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docs citations

11  
times ranked

227  
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular simulation of thermodynamic and transport properties for the H <sub>2</sub> O+NaCl system. Journal of Chemical Physics, 2014, 141, 234507.	3.0	63
2	Atomistic molecular dynamics simulations of H <sub>2</sub> O diffusivity in liquid and supercritical CO <sub>2</sub> . Molecular Physics, 2015, 113, 2805-2814.	1.7	38
3	Optimization of Intermolecular Potential Parameters for the CO <sub>2</sub> /H <sub>2</sub> O Mixture. Journal of Physical Chemistry B, 2014, 118, 11504-11511.	2.6	35
4	A Transferable Force Field for Primary, Secondary, and Tertiary Alkanolamines. Journal of Chemical Theory and Computation, 2013, 9, 2097-2103.	5.3	26
5	Transferable Force Field for Equilibrium and Transport Properties in Linear, Branched, and Bifunctional Amines I. Primary Amines. Journal of Physical Chemistry B, 2011, 115, 14617-14625.	2.6	23
6	Transferable Force Field for Equilibrium and Transport Properties in Linear and Branched Monofunctional and Multifunctional Amines. II. Secondary and Tertiary Amines. Journal of Physical Chemistry B, 2012, 116, 6193-6202.	2.6	18
7	A molecular simulation study of aqueous solutions of amines and alkanolamines: mixture properties and structural analysis. Molecular Simulation, 2014, 40, 123-133.	2.0	16
8	Self-diffusion coefficients of amines, a molecular dynamics study. Fluid Phase Equilibria, 2022, 553, 113301.	2.5	8
9	Equilibrium and Transport Properties of Primary, Secondary and Tertiary Amines by Molecular Simulation. Oil and Gas Science and Technology, 2014, 69, 833-849.	1.4	7
10	Physical Absorption of Green House Gases in Amines: The Influence of Functionality, Structure, and Cross-Interactions. Journal of Physical Chemistry B, 2016, 120, 13136-13143.	2.6	7
11	Predictions of fluidities of amines by molecular simulations: TraPPE-EH vs. OPLS-AA. Fluid Phase Equilibria, 2018, 464, 40-46.	2.5	4