

# Jelle Vekeman

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/781892/publications.pdf>

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16  
papers

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citations

1306789

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1125271

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16  
times ranked

160  
citing authors

#	ARTICLE	IF	CITATIONS
1	Modeling the Interaction of Carbon Monoxide with Flexible Graphene: From Coupled Cluster Calculations to Molecular Dynamics Simulations. <i>ChemPhysChem</i> , 2018, 19, 774-783.	1.0	23
2	Potential models for the simulation of methane adsorption on graphene: development and CCSD(T) benchmarks. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 25518-25530.	1.3	23
3	One Step Further in the Elucidation of the Crystallographic Structure of Whitlockite. <i>Crystal Growth and Design</i> , 2020, 20, 2553-2561.	1.4	18
4	Unravelling phosphate adsorption on hydrous ferric oxide surfaces at the molecular level. <i>Chemosphere</i> , 2020, 261, 127776.	4.2	17
5	Morphology of Calcium Oxalate Polyhydrates: A Quantum Chemical and Computational Study. <i>Crystal Growth and Design</i> , 2020, 20, 3807-3815.	1.4	17
6	Flexibility in the Graphene Sheet: The Influence on Gas Adsorption from Molecular Dynamics Studies. <i>Journal of Physical Chemistry C</i> , 2019, 123, 28035-28047.	1.5	14
7	Molecular Dynamics of CH <sub>4</sub> /N <sub>2</sub> Mixtures on a Flexible Graphene Layer: Adsorption and Selectivity Case Study. <i>Frontiers in Chemistry</i> , 2019, 7, 386.	1.8	14
8	In Search of an Efficient Complexing Agent for Oxalates and Phosphates: A Quantum Chemical Study. <i>Nanomaterials</i> , 2021, 11, 1763.	1.9	8
9	Opportunities given by density functional theory in pathological calcifications. <i>Comptes Rendus Chimie</i> , 2022, 25, 209-218.	0.2	7
10	Towards a predictive model for polymer solubility using the noncovalent interaction index: polyethylene as a case study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25374-25387.	1.3	6
11	Lanthanum carbonate to control plasma and urinary oxalate level in type 1 primary hyperoxaluria?. <i>IJU Case Reports</i> , 2021, 4, 235-238.	0.1	5
12	Grand Canonical Monte Carlo Simulations to Determine the Optimal Interlayer Distance of a Graphene Slit-Shaped Pore for Adsorption of Methane, Hydrogen and their Equimolar Mixture. <i>Nanomaterials</i> , 2021, 11, 2534.	1.9	5
13	A subtle balance between interchain interactions and surface reconstruction at the origin of the alkythiol/Au(111) self-assembled monolayer geometry. <i>Surface Science</i> , 2020, 696, 121597.	0.8	4
14	Nitrogen Gas on Graphene: Pairwise Interaction Potentials. <i>Lecture Notes in Computer Science</i> , 2018, , 563-578.	1.0	3
15	Modeling of Complex Interfaces: From Surface Chemistry to Nano Chemistry. <i>Nanomaterials</i> , 2020, 10, 540.	1.9	2
16	Study on the biological behaviors of Ca P coatings with different morphology on carbon/carbon composites. <i>Materials Science and Engineering C</i> , 2021, 129, 112391.	3.8	1