

# Jelle Vekeman

## List of Publications by Year in descending order

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

Version: 2024-02-01

16  
papers

167  
citations

1307594

7  
h-index

1125743

13  
g-index

16  
all docs

16  
docs citations

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. ChemPhysChem, 2018, 19, 774-783.   | 2.1 | 23        |
| 2  | Potential models for the simulation of methane adsorption on graphene: development and CCSD(T) benchmarks. Physical Chemistry Chemical Physics, 2018, 20, 25518-25530.  | 2.8 | 23        |
| 3  | One Step Further in the Elucidation of the Crystallographic Structure of Whitlockite. Crystal Growth and Design, 2020, 20, 2553-2561.   | 3.0 | 18        |
| 4  | Unravelling phosphate adsorption on hydrous ferric oxide surfaces at the molecular level. Chemosphere, 2020, 261, 127776.   | 8.2 | 17        |
| 5  | Morphology of Calcium Oxalate Polyhydrates: A Quantum Chemical and Computational Study. Crystal Growth and Design, 2020, 20, 3807-3815.   | 3.0 | 17        |
| 6  | Flexibility in the Graphene Sheet: The Influence on Gas Adsorption from Molecular Dynamics Studies. Journal of Physical Chemistry C, 2019, 123, 28035-28047.  | 3.1 | 14        |
| 7  | Molecular Dynamics of CH <sub>4</sub> /N <sub>2</sub> Mixtures on a Flexible Graphene Layer: Adsorption and Selectivity Case Study. Frontiers in Chemistry, 2019, 7, 386.   | 3.6 | 14        |
| 8  | In Search of an Efficient Complexing Agent for Oxalates and Phosphates: A Quantum Chemical Study. Nanomaterials, 2021, 11, 1763.  | 4.1 | 8         |
| 9  | Opportunities given by density functional theory in pathological calcifications. Comptes Rendus Chimie, 2022, 25, 209-218.  | 0.5 | 7         |
| 10 | Towards a predictive model for polymer solubility using the noncovalent interaction index: polyethylene as a case study. Physical Chemistry Chemical Physics, 2021, 23, 25374-25387.                                | 2.8 | 6         |
| 11 | Lanthanum carbonate to control plasma and urinary oxalate level in type 1 primary hyperoxaluria?. IJU Case Reports, 2021, 4, 235-238.   | 0.3 | 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. Nanomaterials, 2021, 11, 2534. | 4.1 | 5         |
| 13 | A subtle balance between interchain interactions and surface reconstruction at the origin of the alkythiol/Au(111) self-assembled monolayer geometry. Surface Science, 2020, 696, 121597.                           | 1.9 | 4         |
| 14 | Nitrogen Gas on Graphene: Pairwise Interaction Potentials. Lecture Notes in Computer Science, 2018, , 563-578.  | 1.3 | 3         |
| 15 | Modeling of Complex Interfaces: From Surface Chemistry to Nano Chemistry. Nanomaterials, 2020, 10, 540.   | 4.1 | 2         |
| 16 | Study on the biological behaviors of Ca P coatings with different morphology on carbon/carbon composites. Materials Science and Engineering C, 2021, 129, 112391.   | 7.3 | 1         |