Jelle Vekeman

List of Publications by Year
in descending order

16	167	1306789 7	1125271 13
papers	citations	h-index	g-index

16	16	16	160
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Opportunities given by density functional theory in pathological calcifications. Comptes Rendus Chimie, 2022, 25, 209-218.	0.2	7
2	Lanthanum carbonate to control plasma and urinary oxalate level in type 1 primary hyperoxaluria?. IJU Case Reports, 2021, 4, 235-238.	0.1	5
3	In Search of an Efficient Complexing Agent for Oxalates and Phosphates: A Quantum Chemical Study. Nanomaterials, 2021, 11, 1763.	1.9	8
4	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.	1.9	5
5	Study on the biological behaviors of Ca P coatings with different morphology on carbon/carbon composites. Materials Science and Engineering C, 2021, 129, 112391.	3.8	1
6	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.	1.3	6
7	Unravelling phosphate adsorption on hydrous ferric oxide surfaces at the molecular level. Chemosphere, 2020, 261, 127776.	4.2	17
8	Modeling of Complex Interfaces: From Surface Chemistry to Nano Chemistry. Nanomaterials, 2020, 10, 540.	1.9	2
9	One Step Further in the Elucidation of the Crystallographic Structure of Whitlockite. Crystal Growth and Design, 2020, 20, 2553-2561.	1.4	18
10	A subtle balance between interchain interactions and surface reconstruction at the origin of the alkylthiol/Au(111) self-assembled monolayer geometry. Surface Science, 2020, 696, 121597.	0.8	4
11	Morphology of Calcium Oxalate Polyhydrates: A Quantum Chemical and Computational Study. Crystal Growth and Design, 2020, 20, 3807-3815.	1.4	17
12	Flexibility in the Graphene Sheet: The Influence on Gas Adsorption from Molecular Dynamics Studies. Journal of Physical Chemistry C, 2019, 123, 28035-28047.	1.5	14
13	Molecular Dynamics of CH4/N2 Mixtures on a Flexible Graphene Layer: Adsorption and Selectivity Case Study. Frontiers in Chemistry, 2019, 7, 386.	1.8	14
14	Modeling the Interaction of Carbon Monoxide with Flexible Graphene: From Coupled Cluster Calculations to Molecularâ€Dynamics Simulations. ChemPhysChem, 2018, 19, 774-783.	1.0	23
15	Potential models for the simulation of methane adsorption on graphene: development and CCSD(T) benchmarks. Physical Chemistry Chemical Physics, 2018, 20, 25518-25530.	1.3	23
16	Nitrogen Gas on Graphene: Pairwise Interaction Potentials. Lecture Notes in Computer Science, 2018, , 563-578.	1.0	3