

Martinus Antonius Zwijnenburg

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

81
papers

4,359
citations

30
h-index

65
g-index

137
ext. papers

5,389
ext. citations

8.7
avg, IF

5.9
L-index

#	Paper	IF	Citations
81	Time-Resolved Raman Spectroscopy of Polaron Formation in a Polymer Photocatalyst. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 10899-10905	6.4	2
80	The Role of Computational Chemistry in Discovering and Understanding Organic Photocatalysts for Renewable Fuel Synthesis. <i>Advanced Energy Materials</i> , 2021 , 11, 2100709	21.8	3
79	Using high-throughput virtual screening to explore the optoelectronic property space of organic dyes; finding diketopyrrolopyrrole dyes for dye-sensitized water splitting and solar cells. <i>Sustainable Energy and Fuels</i> , 2021 , 5, 704-719	5.8	9
78	The effect of particle size on the optical and electronic properties of magnesium oxide nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 21579-21590	3.6	1
77	Acetylene-linked conjugated polymers for sacrificial photocatalytic hydrogen evolution from water. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 17242-17248	13	5
76	Hydrogen evolution by polymer photocatalysts; a possible photocatalytic cycle. <i>Sustainable Energy and Fuels</i> , 2021 , 5, 2622-2632	5.8	4
75	Photocatalytic syngas production using conjugated organic polymers. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 4291-4296	13	13
74	Photocatalytic polymers of intrinsic microporosity for hydrogen production from water. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 19958-19964	13	11
73	Side-chain tuning in conjugated polymer photocatalysts for improved hydrogen production from water. <i>Energy and Environmental Science</i> , 2020 , 13, 1843-1855	35.4	51
72	Controlling the Thermoelectric Properties of Organometallic Coordination Polymers via Ligand Design. <i>Advanced Functional Materials</i> , 2020 , 30, 2003106	15.6	6
71	Molecular generation targeting desired electronic properties via deep generative models. <i>Nanoscale</i> , 2020 , 12, 6744-6758	7.7	16
70	Photocatalytic proton reduction by a computationally identified, molecular hydrogen-bonded framework. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 7158-7170	13	26
69	Hydrogen evolution from water using heteroatom substituted fluorene conjugated co-polymers. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 8700-8705	13	26
68	Water Oxidation with Cobalt-Loaded Linear Conjugated Polymer Photocatalysts. <i>Angewandte Chemie</i> , 2020 , 132, 18854-18859	3.6	6
67	Water Oxidation with Cobalt-Loaded Linear Conjugated Polymer Photocatalysts. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 18695-18700	16.4	24
66	Mapping the optoelectronic property space of small aromatic molecules. <i>Communications Chemistry</i> , 2020 , 3,	6.3	4
65	Photocatalyst Z-scheme system composed of a linear conjugated polymer and BiVO ₄ for overall water splitting under visible light. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 16283-16290	13	32

64	Structure-activity relationships in well-defined conjugated oligomer photocatalysts for hydrogen production from water. <i>Chemical Science</i> , 2020 , 11, 8744-8756	9.4	21
63	Color Differences Highlight Concomitant Polymorphism of Chalcones. <i>Crystal Growth and Design</i> , 2020 , 20, 6346-6355	3.5	5
62	Current understanding and challenges of solar-driven hydrogen generation using polymeric photocatalysts. <i>Nature Energy</i> , 2019 , 4, 746-760	62.3	326
61	Structurally Diverse Covalent Triazine-Based Framework Materials for Photocatalytic Hydrogen Evolution from Water. <i>Chemistry of Materials</i> , 2019 , 31, 8830-8838	9.6	62
60	Computational high-throughput screening of polymeric photocatalysts: exploring the effect of composition, sequence isomerism and conformational degrees of freedom. <i>Faraday Discussions</i> , 2019 , 215, 98-110	3.6	8
59	Photocatalytically active ladder polymers. <i>Faraday Discussions</i> , 2019 , 215, 84-97	3.6	16
58	Biological approaches to artificial photosynthesis: general discussion. <i>Faraday Discussions</i> , 2019 , 215, 66-83	3.6	
57	Demonstrator devices for artificial photosynthesis: general discussion. <i>Faraday Discussions</i> , 2019 , 215, 345-363	3.6	1
56	Synthetic approaches to artificial photosynthesis: general discussion. <i>Faraday Discussions</i> , 2019 , 215, 242-281	3.6	4
55	Accelerated Discovery of Organic Polymer Photocatalysts for Hydrogen Evolution from Water through the Integration of Experiment and Theory. <i>Journal of the American Chemical Society</i> , 2019 , 141, 9063-9071	16.4	156
54	Mapping binary copolymer property space with neural networks. <i>Chemical Science</i> , 2019 , 10, 4973-4984	9.4	24
53	Insight into the self-assembly of water-soluble perylene bisimide derivatives through a combined computational and experimental approach. <i>Nanoscale</i> , 2019 , 11, 15917-15928	7.7	8
52	Photocatalytic Hydrogen Evolution from Water Using Fluorene and Dibenzothiophene Sulfone-Conjugated Microporous and Linear Polymers. <i>Chemistry of Materials</i> , 2019 , 31, 305-313	9.6	116
51	Controlling Photoconductivity in PBI Films by Supramolecular Assembly. <i>Chemistry - A European Journal</i> , 2018 , 24, 4006-4010	4.8	25
50	Nitrogen Containing Linear Poly(phenylene) Derivatives for Photo-catalytic Hydrogen Evolution from Water. <i>Chemistry of Materials</i> , 2018 , 30, 5733-5742	9.6	66
49	Synthesis Target Structures for Alkaline Earth Oxide Clusters. <i>Inorganics</i> , 2018 , 6, 29	2.9	10
48	Maximising the hydrogen evolution activity in organic photocatalysts by co-polymerisation. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 11994-12003	13	73
47	Understanding structure-activity relationships in linear polymer photocatalysts for hydrogen evolution. <i>Nature Communications</i> , 2018 , 9, 4968	17.4	153

46	Sulfone-containing covalent organic frameworks for photocatalytic hydrogen evolution from water. <i>Nature Chemistry</i> , 2018 , 10, 1180-1189	17.6	526
45	High-Throughput Screening Approach for the Optoelectronic Properties of Conjugated Polymers. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 2450-2459	6.1	30
44	Structure prediction of (BaO) _n nanoclusters for n≥24 using an evolutionary algorithm. <i>Computational and Theoretical Chemistry</i> , 2017 , 1107, 74-81	2	11
43	Structure-property relationships for covalent triazine-based frameworks: The effect of spacer length on photocatalytic hydrogen evolution from water. <i>Polymer</i> , 2017 , 126, 283-290	3.9	106
42	pH-Directed Aggregation to Control Photoconductivity in Self-Assembled Perylene Bisimides. <i>Chem</i> , 2017 , 2, 716-731	16.2	40
41	Time-Resolved Spectroscopic Investigation of Charge Trapping in Carbon Nitrides Photocatalysts for Hydrogen Generation. <i>Journal of the American Chemical Society</i> , 2017 , 139, 5216-5224	16.4	307
40	Validating a Density Functional Theory Approach for Predicting the Redox Potentials Associated with Charge Carriers and Excitons in Polymeric Photocatalysts. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 1498-1506	3.8	32
39	Mechanism of photocatalytic water oxidation on small TiO nanoparticles. <i>Chemical Science</i> , 2017 , 8, 2179-2183	5.0	50
38	Benchmarking the Fundamental Electronic Properties of small TiO Nanoclusters by GW and Coupled Cluster Theory Calculations. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 3814-3828	6.4	15
37	Reversible Photoreduction as a Trigger for Photoresponsive Gels. <i>Chemistry of Materials</i> , 2016 , 28, 6336-6341	6.4	30
36	Modelling materials for solar fuel synthesis by artificial photosynthesis; predicting the optical, electronic and redox properties of photocatalysts. <i>Journal of Physics Condensed Matter</i> , 2016 , 28, 074001	1.8	11
35	Visible-Light-Driven Hydrogen Evolution Using Planarized Conjugated Polymer Photocatalysts. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 1792-6	16.4	288
34	Visible-Light-Driven Hydrogen Evolution Using Planarized Conjugated Polymer Photocatalysts. <i>Angewandte Chemie</i> , 2016 , 128, 1824-1828	3.6	133
33	Amine Molecular Cages as Supramolecular Fluorescent Explosive Sensors: A Computational Perspective. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 5063-72	3.4	24
32	Controlling Visible Light Driven Photoconductivity in Self-Assembled Perylene Bisimide Structures. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 18479-18486	3.8	30
31	Polymer Photocatalysts for Water Splitting: Insights from Computational Modeling. <i>Macromolecular Chemistry and Physics</i> , 2016 , 217, 344-353	2.6	60
30	Contrasting the optical properties of the different isomers of oligophenylene. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 17854-63	3.6	19
29	Chemical trends in the optical properties of rocksalt nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 28892-900	3.6	9

28	Modeling the Water Splitting Activity of a TiO ₂ Rutile Nanoparticle. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 13384-13393	3.8	30
27	Tunable organic photocatalysts for visible-light-driven hydrogen evolution. <i>Journal of the American Chemical Society</i> , 2015 , 137, 3265-70	16.4	611
26	Describing Excited State Relaxation and Localization in TiO ₂ Nanoparticles Using TD-DFT. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 5538-48	6.4	29
25	Optical excitation of MgO nanoparticles; a computational perspective. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 22052-61	3.6	28
24	Polymeric watersplitting photocatalysts; a computational perspective on the water oxidation conundrum. <i>Journal of Materials Chemistry A</i> , 2014 , 2, 11996-12004	13	48
23	Air-stable photoconductive films formed from perylene bisimide gelators. <i>Journal of Materials Chemistry C</i> , 2014 , 2, 5570-5575	7.1	70
22	Shining a Light on s-Triazine-Based Polymers. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 4314-4324	3.8	38
21	Modeling Excited States in TiO Nanoparticles: On the Accuracy of a TD-DFT Based Description. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 1189-1199	6.4	48
20	Carbon Nitride Photocatalysts for Water Splitting: A Computational Perspective. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 24833-24842	3.8	88
19	Shedding Light on Structure-Property Relationships for Conjugated Microporous Polymers: The Importance of Rings and Strain. <i>Macromolecules</i> , 2013 , 46, 7696-7704	5.5	39
18	Excited state localisation cascades in inorganic semiconductor nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 11119-27	3.6	11
17	Coupled cluster calculations on TiO ₂ nanoclusters. <i>Journal of Chemical Physics</i> , 2013 , 139, 064313	3.9	12
16	Elucidating the Microscopic Origin of the Unique Optical Properties of Polypyrene. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 20191-20198	3.8	5
15	Photoluminescence in semiconductor nanoparticles: an atomistic view of excited state relaxation in nanosized ZnS. <i>Nanoscale</i> , 2012 , 4, 3711-7	7.7	19
14	The fate of optical excitations in small polyhedral ZnS clusters: a theoretical study of the excitation and localization of electrons in Zn ₄ S ₄ and Zn ₆ S ₆ . <i>Journal of Chemical Physics</i> , 2011 , 134, 064511	3.9	18
13	Optical excitations in stoichiometric uncapped ZnS nanostructures. <i>Nanoscale</i> , 2011 , 3, 3780-7	7.7	19
12	Structure direction in zinc oxide and related materials by cation substitution: an analogy with zeolites. <i>Journal of Materials Chemistry</i> , 2011 , 21, 15255		13
11	The fate of optical excitations in small hydrated ZnS clusters: a theoretical study into the effect of hydration on the excitation and localisation of electrons in Zn ₄ S ₄ and Zn ₆ S ₆ . <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 9311-7	3.6	18

10	Structural richness of ionic binary materials: An exploration of the energy landscape of magnesium oxide. <i>Physical Review B</i> , 2011 , 83,	3.3	22
9	Isomorphism between ice and silica. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 8597-606	3.6	36
8	Isomorphism of anhydrous tetrahedral halides and silicon chalcogenides: energy landscape of crystalline BeF ₂ , BeCl ₂ , SiO ₂ , and SiS ₂ . <i>Journal of the American Chemical Society</i> , 2008 , 130, 11082-7	16.4	16
7	Absence of Limitations on the Framework Density and Pore Size of High-Silica Zeolites. <i>Chemistry of Materials</i> , 2008 , 20, 3008-3014	9.6	18
6	Going beyond SiO ₂ and AlPO ₄ : Stabilisation of strained hypothetical frameworks in exotic compositions. <i>Studies in Surface Science and Catalysis</i> , 2008 , 174, 695-700	1.8	
5	Structure, bonding and physical properties of tetragonal and orthorhombic SiS ₂ from (hybrid) DFT calculations. <i>Journal of Solid State Chemistry</i> , 2008 , 181, 2480-2487	3.3	11
4	Dramatic differences between the energy landscapes of SiO(2) and SiS(2) zeotype materials. <i>Journal of the American Chemical Society</i> , 2007 , 129, 12588-9	16.4	16
3	A computational study into the (tetrahedral) distortion of TX ₂ quartz materials: The effect of changing the chemical composition away from SiO ₂ . <i>Journal of Solid State Chemistry</i> , 2006 , 179, 3429-3436	3.3	17
2	Comparing the influence of framework type on H ₂ absorption in hypothetical and existing clathrasils: a grand canonical Monte Carlo study. <i>Journal of Materials Chemistry</i> , 2006 , 16, 3285		6
1	Tetrahedral distortion and energetic packing penalty in "zeolite" frameworks: linked phenomena?. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 14783-5	3.4	24