Martinus Antonius Zwijnenburg

List of Publications by Citations

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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	Tunable organic photocatalysts for visible-light-driven hydrogen evolution. *Journal of the American Chemical Society*, **2015**, 137, 3265-70	16.4	611
80	Sulfone-containing covalent organic frameworks for photocatalytic hydrogen evolution from water. *Nature Chemistry*, **2018**, 10, 1180-1189	17.6	526
79	Current understanding and challenges of solar-driven hydrogen generation using polymeric photocatalysts. *Nature Energy*, **2019**, 4, 746-760	62.3	326
78	Time-Resolved Spectroscopic Investigation of Charge Trapping in Carbon Nitrides Photocatalysts for Hydrogen Generation. *Journal of the American Chemical Society*, **2017**, 139, 5216-5224	16.4	307
77	Visible-Light-Driven Hydrogen Evolution Using Planarized Conjugated Polymer Photocatalysts. *Angewandte Chemie - International Edition*, **2016**, 55, 1792-6	16.4	288
76	Accelerated Discovery of Organic Polymer Photocatalysts for Hydrogen Evolution from Water through the Integration of Experiment and Theory. *Journal of the American Chemical Society*, **2019**, 141, 9063-9071	16.4	156
75	Understanding structure-activity relationships in linear polymer photocatalysts for hydrogen evolution. *Nature Communications*, **2018**, 9, 4968	17.4	153
74	Visible-Light-Driven Hydrogen Evolution Using Planarized Conjugated Polymer Photocatalysts. *Angewandte Chemie*, **2016**, 128, 1824-1828	3.6	133
73	Photocatalytic Hydrogen Evolution from Water Using Fluorene and Dibenzothiophene Sulfone-Conjugated Microporous and Linear Polymers. *Chemistry of Materials*, **2019**, 31, 305-313	9.6	116
72	Structure-property relationships for covalent triazine-based frameworks: The effect of spacer length on photocatalytic hydrogen evolution from water. *Polymer*, **2017**, 126, 283-290	3.9	106
71	Carbon Nitride Photocatalysts for Water Splitting: A Computational Perspective. *Journal of Physical Chemistry C*, **2014**, 118, 24833-24842	3.8	88
70	Maximising the hydrogen evolution activity in organic photocatalysts by co-polymerisation. *Journal of Materials Chemistry A*, **2018**, 6, 11994-12003	13	73
69	Air-stable photoconductive films formed from perylene bisimide gelators. *Journal of Materials Chemistry C*, **2014**, 2, 5570-5575	7.1	70
68	Nitrogen Containing Linear Poly(phenylene) Derivatives for Photo-catalytic Hydrogen Evolution from Water. *Chemistry of Materials*, **2018**, 30, 5733-5742	9.6	66
67	Structurally Diverse Covalent Triazine-Based Framework Materials for Photocatalytic Hydrogen Evolution from Water. *Chemistry of Materials*, **2019**, 31, 8830-8838	9.6	62
66	Polymer Photocatalysts for Water Splitting: Insights from Computational Modeling. *Macromolecular Chemistry and Physics*, **2016**, 217, 344-353	2.6	60
65	Side-chain tuning in conjugated polymer photocatalysts for improved hydrogen production from water. *Energy and Environmental Science*, **2020**, 13, 1843-1855	35.4	51

64	Mechanism of photocatalytic water oxidation on small TiO nanoparticles. *Chemical Science*, **2017**, 8, 2179-2183	9.4	50
63	Polymeric watersplitting photocatalysts; a computational perspective on the water oxidation conundrum. *Journal of Materials Chemistry A*, **2014**, 2, 11996-12004	13	48
62	Modeling Excited States in TiO Nanoparticles: On the Accuracy of a TD-DFT Based Description. *Journal of Chemical Theory and Computation*, **2014**, 10, 1189-1199	6.4	48
61	pH-Directed Aggregation to Control Photoconductivity in Self-Assembled Perylene Bisimides. *CheM* , **2017**, 2, 716-731	16.2	40
60	Shedding Light on Structure-Property Relationships for Conjugated Microporous Polymers: The Importance of Rings and Strain. *Macromolecules*, **2013**, 46, 7696-7704	5.5	39
59	Shining a Light on s-Triazine-Based Polymers. *Journal of Physical Chemistry C*, **2014**, 118, 4314-4324	3.8	38
58	Isomorphism between ice and silica. *Physical Chemistry Chemical Physics*, **2010**, 12, 8597-606	3.6	36
57	Validating a Density Functional Theory Approach for Predicting the Redox Potentials Associated with Charge Carriers and Excitons in Polymeric Photocatalysts. *Journal of Physical Chemistry C*, **2017** , 121, 1498-1506	3.8	32
56	Photocatalyst Z-scheme system composed of a linear conjugated polymer and $BiVO_4$ for overall water splitting under visible light. *Journal of Materials Chemistry A*, **2020**, 8, 16283-16290	13	32
55	Reversible Photoreduction as a Trigger for Photoresponsive Gels. *Chemistry of Materials*, **2016**, 28, 6336-6341	9.7	30
54	Modeling the Water Splitting Activity of a TiO_2 Rutile Nanoparticle. *Journal of Physical Chemistry C*, **2015**, 119, 13384-13393	3.8	30
53	Controlling Visible Light Driven Photoconductivity in Self-Assembled Perylene Bisimide Structures. *Journal of Physical Chemistry C*, **2016**, 120, 18479-18486	3.8	30
52	High-Throughput Screening Approach for the Optoelectronic Properties of Conjugated Polymers. *Journal of Chemical Information and Modeling*, **2018**, 58, 2450-2459	6.1	30
51	Describing Excited State Relaxation and Localization in TiO_2 Nanoparticles Using TD-DFT. *Journal of Chemical Theory and Computation*, **2014**, 10, 5538-48	6.4	29
50	Optical excitation of MgO nanoparticles; a computational perspective. *Physical Chemistry Chemical Physics*, **2014**, 16, 22052-61	3.6	28
49	Photocatalytic proton reduction by a computationally identified, molecular hydrogen-bonded framework. *Journal of Materials Chemistry A*, **2020**, 8, 7158-7170	13	26
48	Hydrogen evolution from water using heteroatom substituted fluorene conjugated co-polymers. *Journal of Materials Chemistry A*, **2020**, 8, 8700-8705	13	26
47	Controlling Photoconductivity in PBI Films by Supramolecular Assembly. *Chemistry - A European Journal*, **2018**, 24, 4006-4010	4.8	25

46	Mapping binary copolymer property space with neural networks. *Chemical Science*, **2019**, 10, 4973-4984	9.4	24
45	Water Oxidation with Cobalt-Loaded Linear Conjugated Polymer Photocatalysts. *Angewandte Chemie - International Edition*, **2020**, 59, 18695-18700	16.4	24
44	Tetrahedral distortion and energetic packing penalty in "zeolite" frameworks: linked phenomena?. *Journal of Physical Chemistry B*, **2005**, 109, 14783-5	3.4	24
43	Amine Molecular Cages as Supramolecular Fluorescent Explosive Sensors: A Computational Perspective. *Journal of Physical Chemistry B*, **2016**, 120, 5063-72	3.4	24
42	Structural richness of ionic binary materials: An exploration of the energy landscape of magnesium oxide. *Physical Review B*, **2011**, 83,	3.3	22
41	Structure-activity relationships in well-defined conjugated oligomer photocatalysts for hydrogen production from water. *Chemical Science*, **2020**, 11, 8744-8756	9.4	21
40	Contrasting the optical properties of the different isomers of oligophenylene. *Physical Chemistry Chemical Physics*, **2015**, 17, 17854-63	3.6	19
39	Photoluminescence in semiconductor nanoparticles: an atomistic view of excited state relaxation in nanosized ZnS. *Nanoscale*, **2012**, 4, 3711-7	7.7	19
38	Optical excitations in stoichiometric uncapped ZnS nanostructures. *Nanoscale*, **2011**, 3, 3780-7	7.7	19
37	The fate of optical excitations in small polyhedral ZnS clusters: a theoretical study of the excitation and localization of electrons in Zn4S4 and Zn6S6. *Journal of Chemical Physics*, **2011**, 134, 064511	3.9	18
36	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 Zn4S4 and Zn6S6. *Physical Chemistry Chemical Physics*, **2011**, 13, 9311-7	3.6	18
35	Absence of Limitations on the Framework Density and Pore Size of High-Silica Zeolites. *Chemistry of Materials*, **2008**, 20, 3008-3014	9.6	18
34	A computational study into the (tetrahedral) distortion of TX2 -quartz materials: The effect of changing the chemical composition away from SiO2. *Journal of Solid State Chemistry*, **2006**, 179, 3429-3436	3.3	17
33	Photocatalytically active ladder polymers. *Faraday Discussions*, **2019**, 215, 84-97	3.6	16
32	Molecular generation targeting desired electronic properties via deep generative models. *Nanoscale*, **2020**, 12, 6744-6758	7.7	16
31	Isomorphism of anhydrous tetrahedral halides and silicon chalcogenides: energy landscape of crystalline BeF2, BeCl2, SiO2, and SiS2. *Journal of the American Chemical Society*, **2008**, 130, 11082-7	16.4	16
30	Dramatic differences between the energy landscapes of SiO(2) and SiS(2) zeotype materials. *Journal of the American Chemical Society*, **2007**, 129, 12588-9	16.4	16
29	Benchmarking the Fundamental Electronic Properties of small TiO Nanoclusters by GW and Coupled Cluster Theory Calculations. *Journal of Chemical Theory and Computation*, **2017**, 13, 3814-3828	6.4	15

28	Structure direction in zinc oxide and related materials by cation substitution: an analogy with zeolites. *Journal of Materials Chemistry*, **2011**, 21, 15255		13
27	Photocatalytic syngas production using conjugated organic polymers. *Journal of Materials Chemistry A*, **2021**, 9, 4291-4296	13	13
26	Coupled cluster calculations on TiO2 nanoclusters. *Journal of Chemical Physics*, **2013**, 139, 064313	3.9	12
25	Structure prediction of (BaO)n nanoclusters for n?24 using an evolutionary algorithm. *Computational and Theoretical Chemistry*, **2017**, 1107, 74-81	2	11
24	Excited state localisation cascades in inorganic semiconductor nanoparticles. *Physical Chemistry Chemical Physics*, **2013**, 15, 11119-27	3.6	11
23	Structure, bonding and physical properties of tetragonal and orthorhombic SiS2 from (hybrid) DFT calculations. *Journal of Solid State Chemistry*, **2008**, 181, 2480-2487	3.3	11
22	Modelling materials for solar fuel synthesis by artificial photosynthesis; predicting the optical, electronic and redox properties of photocatalysts. *Journal of Physics Condensed Matter*, **2016**, 28, 074001	1.8	11
21	Photocatalytic polymers of intrinsic microporosity for hydrogen production from water. *Journal of Materials Chemistry A*, **2021**, 9, 19958-19964	13	11
20	Synthesis Target Structures for Alkaline Earth Oxide Clusters. *Inorganics*, **2018**, 6, 29	2.9	10
19	Chemical trends in the optical properties of rocksalt nanoparticles. *Physical Chemistry Chemical Physics*, **2015**, 17, 28892-900	3.6	9
18	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. *Sustainable Energy and Fuels*, **2021**, 5, 704-719	5.8	9
17	Computational high-throughput screening of polymeric photocatalysts: exploring the effect of composition, sequence isomerism and conformational degrees of freedom. *Faraday Discussions*, **2019**, 215, 98-110	3.6	8
16	Insight into the self-assembly of water-soluble perylene bisimide derivatives through a combined computational and experimental approach. *Nanoscale*, **2019**, 11, 15917-15928	7.7	8
15	Controlling the Thermoelectric Properties of Organometallic Coordination Polymers via Ligand Design. *Advanced Functional Materials*, **2020**, 30, 2003106	15.6	6
14	Water Oxidation with Cobalt-Loaded Linear Conjugated Polymer Photocatalysts. *Angewandte Chemie*, **2020**, 132, 18854-18859	3.6	6
13	Comparing the influence of framework type on H2 absorption in hypothetical and existing clathrasils: a grand canonical Monte Carlo study. *Journal of Materials Chemistry*, **2006**, 16, 3285		6
12	Elucidating the Microscopic Origin of the Unique Optical Properties of Polypyrene. *Journal of Physical Chemistry C*, **2012**, 116, 20191-20198	3.8	5
11	Color Differences Highlight Concomitant Polymorphism of Chalcones. *Crystal Growth and Design*, **2020**, 20, 6346-6355	3.5	5

10	Acetylene-linked conjugated polymers for sacrificial photocatalytic hydrogen evolution from water. *Journal of Materials Chemistry A*, **2021**, 9, 17242-17248	13	5
9	Synthetic approaches to artificial photosynthesis: general discussion. *Faraday Discussions*, **2019**, 215, 242-281	3.6	4
8	Mapping the optoelectronic property space of small aromatic molecules. *Communications Chemistry*, **2020**, 3,	6.3	4
7	Hydrogen evolution by polymer photocatalysts; a possible photocatalytic cycle. *Sustainable Energy and Fuels*, **2021**, 5, 2622-2632	5.8	4
6	The Role of Computational Chemistry in Discovering and Understanding Organic Photocatalysts for Renewable Fuel Synthesis. *Advanced Energy Materials*, **2021**, 11, 2100709	21.8	3
5	Time-Resolved Raman Spectroscopy of Polaron Formation in a Polymer Photocatalyst. *Journal of Physical Chemistry Letters*, **2021**, 12, 10899-10905	6.4	2
4	Demonstrator devices for artificial photosynthesis: general discussion. *Faraday Discussions*, **2019**, 215, 345-363	3.6	1
3	The effect of particle size on the optical and electronic properties of magnesium oxide nanoparticles. *Physical Chemistry Chemical Physics*, **2021**, 23, 21579-21590	3.6	1
2	Biological approaches to artificial photosynthesis: general discussion. *Faraday Discussions*, **2019**, 215, 66-83	3.6	
1	Going beyond SiO2 and AlPO4: Stabilisation of strained hypothetical frameworks in exotic compositions. *Studies in Surface Science and Catalysis*, **2008**, 174, 695-700	1.8	