

Geert Brocks

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/9602018/publications.pdf>

Version: 2024-02-01

49
papers

4,618
citations

257450

24
h-index

223800

46
g-index

51
all docs

51
docs citations

51
times ranked

7100
citing authors

#	ARTICLE	IF	CITATIONS
1	Anti-Ferromagnetic RuO ₂ : A Stable and Robust OER Catalyst over a Large Range of Surface Terminations. <i>Journal of Physical Chemistry C</i> , 2022, 126, 1337-1345.	3.1	21
2	Decomposition of Organic Perovskite Precursors on MoO ₃ : Role of Halogen and Surface Defects. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 34208-34219.	8.0	9
3	A ReaxFF Molecular Dynamics Study of Hydrogen Diffusion in Rutheniumâ€œThe Role of Grain Boundaries. <i>Journal of Physical Chemistry C</i> , 2022, 126, 5950-5959.	3.1	3
4	Intrinsic defects in primary halide perovskites: A first-principles study of the thermodynamic trends. <i>Physical Review Materials</i> , 2022, 6, .	2.4	15
5	Phenylalkylammonium passivation enables perovskite light emitting diodes with record high-radiance operational lifetime: the chain length matters. <i>Nature Communications</i> , 2021, 12, 644.	12.8	109
6	Oxygen evolution reaction (OER) mechanism under alkaline and acidic conditions. <i>JPhys Energy</i> , 2021, 3, 026001.	5.3	121
7	1D metallic states at 2D transition metal dichalcogenide semiconductor heterojunctions. <i>Npj 2D Materials and Applications</i> , 2021, 5, .	7.9	2
8	Unified theory for light-induced halide segregation in mixed halide perovskites. <i>Nature Communications</i> , 2021, 12, 2687.	12.8	70
9	Tailoring the Performance of ZnO for Oxygen Evolution by Effective Transition Metal Doping. <i>ChemSusChem</i> , 2021, 14, 3064-3073.	6.8	9
10	Multifunctional Molecule Engineered SnO ₂ for Perovskite Solar Cells with High Efficiency and Reduced Lead Leakage. <i>Solar Rrl</i> , 2021, 5, 2100464.	5.8	26
11	First-principles calculations of defects in metal halide perovskites: A performance comparison of density functionals. <i>Physical Review Materials</i> , 2021, 5, .	2.4	12
12	One-dimensional electronic instabilities at the edges of MoS ₂ . <i>Physical Review B</i> , 2020, 102, .	3.2	12
13	Spin/charge density waves at the boundaries of transition metal dichalcogenides. <i>Physical Review B</i> , 2020, 102, .	3.2	11
14	Engineering the Phases and Heterostructures of Ultrathin Hybrid Perovskite Nanosheets. <i>Advanced Materials</i> , 2020, 32, e2002392.	21.0	25
15	Precise Control of Perovskite Crystallization Kinetics via Sequential Aâ€œSite Doping. <i>Advanced Materials</i> , 2020, 32, e2004630.	21.0	122
16	Microscopic Degradation in Formamidinium-Cesium Lead Iodide Perovskite Solar Cells under Operational Stressors. <i>Joule</i> , 2020, 4, 1743-1758.	24.0	156
17	Hydrogen diffusion out of rutheniumâ€œan ab initio study of the role of adsorbates. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 7935-7941.	2.8	8
18	Tuning the electronic levels of NiO with alkali halides surface modifiers for perovskite solar cells. <i>Physical Review Materials</i> , 2020, 4, .	2.4	9

#	ARTICLE	IF	CITATIONS
19	Enhanced Incorporation of Guanidinium in Formamidinium-Based Perovskites for Efficient and Stable Photovoltaics: The Role of Cs and Br. <i>Advanced Functional Materials</i> , 2019, 29, 1905739.	14.9	41
20	Monolayer Nitrides Doped with Transition Metals as Efficient Catalysts for Water Oxidation: The Singular Role of Nickel. <i>Journal of Physical Chemistry C</i> , 2019, 123, 26289-26298.	3.1	12
21	Boosting the Performance of $WO_3/n\text{-Si}$ Heterostructures for Photoelectrochemical Water Splitting: from the Role of Si to Interface Engineering. <i>Advanced Energy Materials</i> , 2019, 9, 1900940.	19.5	48
22	Absolute energy level positions in tin- and lead-based halide perovskites. <i>Nature Communications</i> , 2019, 10, 2560.	12.8	381
23	Cation and anion immobilization through chemical bonding enhancement with fluorides for stable halide perovskite solar cells. <i>Nature Energy</i> , 2019, 4, 408-415.	39.5	831
24	Evidence of Spin Frustration in a Vanadium Diselenide Monolayer Magnet. <i>Advanced Materials</i> , 2019, 31, e1901185.	21.0	129
25	First-principles study of van der Waals interactions and lattice mismatch at $\text{MoS}_2/\text{SiO}_2/\text{Si}$ interfaces. <i>Physical Review B</i> , 2016, 93, .	11.2	132
26	Green's function approach to edge states in transition metal dichalcogenides. <i>Physical Review B</i> , 2016, 93, .	3.2	16
27	Ohmic Contacts to 2D Semiconductors through van der Waals Bonding. <i>Advanced Electronic Materials</i> , 2016, 2, 1500405.	5.1	91
28	Controlling the Schottky barrier at $\text{MoS}_2/\text{metal}$ contacts by inserting a BN monolayer. <i>Physical Review B</i> , 2015, 91, .	3.2	172
29	Schottky barriers at hexagonal boron nitride/metal interfaces: A first-principles study. <i>Physical Review B</i> , 2014, 90, .	3.2	87
30	Magnetoresistance in multilayer fullerene spin valves: A first-principles study. <i>Physical Review B</i> , 2014, 90, .	3.2	20
31	Large potential steps at weakly interacting metal-insulator interfaces. <i>Physical Review B</i> , 2014, 90, .	3.2	24
32	From spin-polarized interfaces to giant magnetoresistance in organic spin valves. <i>Physical Review B</i> , 2014, 89, .	3.2	15
33	Magnetic Properties of $\text{bcc-Fe}(001)/\text{C}_{60}$ Interfaces for Organic Spintronics. <i>ACS Applied Materials & Interfaces</i> , 2013, 5, 837-841.	8.0	39
34	Role of intrinsic molecular dipole in energy level alignment at organic interfaces. <i>Applied Physics Letters</i> , 2013, 102, 223301.	3.3	28
35	Modeling charge transfer at organic donor-acceptor semiconductor interfaces. <i>Applied Physics Letters</i> , 2012, 100, 203302.	3.3	27
36	First-Principles Study of LiBH_4 Nanoclusters and Their Hydrogen Storage Properties. <i>Journal of Physical Chemistry C</i> , 2012, 116, 18038-18047.	3.1	23

#	ARTICLE	IF	CITATIONS
37	Electrostatic Doping of Graphene through Ultrathin Hexagonal Boron Nitride Films. Nano Letters, 2011, 11, 4631-4635.	9.1	118
38	Fermi level pinning by integer charge transfer at electrode-organic semiconductor interfaces. Applied Physics Letters, 2011, 98, 113303.	3.3	42
39	First-principles study of the dipole layer formation at metal-organic interfaces. Physical Review B, 2010, 81, .	3.2	48
40	The Formation of Self-Assembled Nanowire Arrays on Ge(001): a DFT Study of Pt Induced Nanowire Arrays. Materials Research Society Symposia Proceedings, 2009, 1177, 19.	0.1	2
41	Tunable hydrogen storage in magnesium-transition metal compounds: First-principles calculations. Physical Review B, 2009, 79, .	3.2	48
42	First-principles calculations of the crystal structure, electronic structure, and thermodynamic stability of Be_2Mg_2 . Physical Review B, 2008, 77, .	3.2	31
43	Formation of Pt-induced Ge atomic nanowires on Pt/Ge(001): A density functional theory study. Physical Review B, 2008, 77, .	3.2	130
44	Substrate-induced band gap in graphene on hexagonal boron nitride: <i>Ab initio</i> density functional calculations. Physical Review B, 2007, 76, .	3.2	1,292
45	Plane-wave calculations applied to conjugated polymers. Theoretical Chemistry Accounts, 2000, 104, 116-122.	1.4	6
46	π -dimers of oligothiophene cations. Journal of Chemical Physics, 2000, 112, 5353-5363.	3.0	45
47	Probing the Chemical Instability of the Perovskite/MoO ₃ Interface via Precursor Studies. , 0, , .		0
48	Structural Phases Modulate Light-Induced Halide Segregation in Lower Dimensional Perovskites. , 0, , .		0
49	Monolayer Nitrides Doped with Transition Metals as Efficient Catalysts for Water Oxidation: the Singular Role of Nickel. , 0, , .		0