Geert Brocks

List of Publications by Year
in descending order

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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	Substrate-induced band gap in graphene on hexagonal boron nitride:Ab initiodensity functional calculations. Physical Review B, 2007, 76, .	3.2	1,292
2	Cation and anion immobilization through chemical bonding enhancement with fluorides for stable halide perovskite solar cells. Nature Energy, 2019, 4, 408-415.	39.5	831
3	Absolute energy level positions in tin- and lead-based halide perovskites. Nature Communications, 2019, 10, 2560.	12.8	381
4	Controlling the Schottky barrier at<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">MoS</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math>/metal contacts by inserting a BN monolayer. Physical Review B, 2015, 91, .	3.2	172
5	Microscopic Degradation in Formamidinium-Cesium Lead Iodide Perovskite Solar Cells under Operational Stressors. Joule, 2020, 4, 1743-1758.	24.0	156
6	First-principles study of van der Waals interactions and lattice mismatch at<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub><mm Physical Review B, 2016, 93, .	3.2	132
7	Formation of Pt-induced Ge atomic nanowires on Pt/Ge(001): A density functional theory study. Physical Review B, 2008, 77, .	3.2	130
8	Evidence of Spin Frustration in a Vanadium Diselenide Monolayer Magnet. Advanced Materials, 2019, 31, e1901185.	21.0	129
9	Precise Control of Perovskite Crystallization Kinetics via Sequential Aâ€Site Doping. Advanced Materials, 2020, 32, e2004630.	21.0	122
10	Oxygen evolution reaction (OER) mechanism under alkaline and acidic conditions. JPhys Energy, 2021, 3, 026001.	5.3	121
11	Electrostatic Doping of Graphene through Ultrathin Hexagonal Boron Nitride Films. Nano Letters, 2011, 11, 4631-4635.	9.1	118
12	Phenylalkylammonium passivation enables perovskite light emitting diodes with record high-radiance operational lifetime: the chain length matters. Nature Communications, 2021, 12, 644.	12.8	109
13	Ohmic Contacts to 2D Semiconductors through van der Waals Bonding. Advanced Electronic Materials, 2016, 2, 1500405.	5.1	91
14	Schottky barriers at hexagonal boron nitride/metal interfaces: A first-principles study. Physical Review B, 2014, 90, .	3.2	87
15	Unified theory for light-induced halide segregation in mixed halide perovskites. Nature Communications, 2021, 12, 2687.	12.8	70
16	Tunable hydrogen storage in magnesiumâ€“transition metal compounds: First-principles calculations. Physical Review B, 2009, 79, .	3.2	48
17	First-principles study of the dipole layer formation at metal-organic interfaces. Physical Review B, 2010, 81, .	3.2	48
18	Boosting the Performance of WO₃/nâ€Si Heterostructures for Photoelectrochemical Water Splitting: from the Role of Si to Interface Engineering. Advanced Energy Materials, 2019, 9, 1900940.	19.5	48

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19	Ï€-dimers of oligothiophene cations. Journal of Chemical Physics, 2000, 112, 5353-5363.	3.0	45
20	Fermi level pinning by integer charge transfer at electrode-organic semiconductor interfaces. Applied Physics Letters, 2011, 98, 113303.	3.3	42
21	Enhanced Incorporation of Guanidinium in Formamidiniumâ€Based Perovskites for Efficient and Stable Photovoltaics: The Role of Cs and Br. Advanced Functional Materials, 2019, 29, 1905739.	14.9	41
22	Magnetic Properties of bcc-Fe(001)/C₆₀ Interfaces for Organic Spintronics. ACS Applied Materials & Interfaces, 2013, 5, 837-841.	8.0	39
23	First-principles calculations of the crystal structure, electronic structure, and thermodynamic stability of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Be</mml:mtext><mml:msub><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mrow> Physical Review B, 2008, 77, .	3.2	31
24	Role of intrinsic molecular dipole in energy level alignment at organic interfaces. Applied Physics Letters, 2013, 102, 223301.	3.3	28
25	Modeling charge transfer at organic donor-acceptor semiconductor interfaces. Applied Physics Letters, 2012, 100, 203302.	3.3	27
26	Multifunctional Molecule Engineered SnO₂ for Perovskite Solar Cells with High Efficiency and Reduced Lead Leakage. Solar Rrl, 2021, 5, 2100464.	5.8	26
27	Engineering the Phases and Heterostructures of Ultrathin Hybrid Perovskite Nanosheets. Advanced Materials, 2020, 32, e2002392.	21.0	25
28	Large potential steps at weakly interacting metal-insulator interfaces. Physical Review B, 2014, 90, .	3.2	24
29	First-Principles Study of LiBH4Nanoclusters and Their Hydrogen Storage Properties. Journal of Physical Chemistry C, 2012, 116, 18038-18047.	3.1	23
30	Anti-Ferromagnetic RuO₂: A Stable and Robust OER Catalyst over a Large Range of Surface Terminations. Journal of Physical Chemistry C, 2022, 126, 1337-1345.	3.1	21
31	Magnetoresistance in multilayer fullerene spin valves: A first-principles study. Physical Review B, 2014, 90, .	3.2	20
32	Green's function approach to edge states in transition metal dichalcogenides. Physical Review B, 2016, 93, .	3.2	16
33	From spin-polarized interfaces to giant magnetoresistance in organic spin valves. Physical Review B, 2014, 89, .	3.2	15
34	Intrinsic defects in primary halide perovskites: A first-principles study of the thermodynamic trends. Physical Review Materials, 2022, 6, .	2.4	15
35	Monolayer Nitrides Doped with Transition Metals as Efficient Catalysts for Water Oxidation: The Singular Role of Nickel. Journal of Physical Chemistry C, 2019, 123, 26289-26298.	3.1	12
36	One-dimensional electronic instabilities at the edges of MoS2. Physical Review B, 2020, 102, .	3.2	12

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37	First-principles calculations of defects in metal halide perovskites: A performance comparison of density functionals. Physical Review Materials, 2021, 5, .	2.4	12
38	Spin/charge density waves at the boundaries of transition metal dichalcogenides. Physical Review B, 2020, 102, .	3.2	11
39	Tailoring the Performance of ZnO for Oxygen Evolution by Effective Transition Metal Doping. ChemSusChem, 2021, 14, 3064-3073.	6.8	9
40	Tuning the electronic levels of NiO with alkali halides surface modifiers for perovskite solar cells. Physical Review Materials, 2020, 4, .	2.4	9
41	Decomposition of Organic Perovskite Precursors on MoO₃: Role of Halogen and Surface Defects. ACS Applied Materials & Interfaces, 2022, 14, 34208-34219.	8.0	9
42	Hydrogen diffusion out of rutheniumâ€"an ab initio study of the role of adsorbates. Physical Chemistry Chemical Physics, 2020, 22, 7935-7941.	2.8	8
43	Plane-wave calculations applied to conjugated polymers. Theoretical Chemistry Accounts, 2000, 104, 116-122.	1.4	6
44	A ReaxFF Molecular Dynamics Study of Hydrogen Diffusion in Rutheniumâ€"The Role of Grain Boundaries. Journal of Physical Chemistry C, 2022, 126, 5950-5959.	3.1	3
45	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
46	1D metallic states at 2D transition metal dichalcogenide semiconductor heterojunctions. Npj 2D Materials and Applications, 2021, 5, .	7.9	2
47	Probing the Chemical Instability of the Perovskite/MoO3 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