Michel Bockstedte

List of Publications by Year
in descending order

74 papers	3,131 citations	218592 26 h-index	155592 55 g-index
75 all docs	75 docs citations	75 times ranked	2460 citing authors

#	Article	IF	Citations
1	Density-functional theory calculations for poly-atomic systems: electronic structure, static and elastic properties and ab initio molecular dynamics. Computer Physics Communications, 1997, 107, 187-222.	3.0	660
2	Ab initiostudy of the migration of intrinsic defects in3Câ”SiC. Physical Review B, 2003, 68, .	1.1	241
3	Pseudopotential study of binding properties of solids within generalized gradient approximations: The role of core-valence exchange correlation. Physical Review B, 1998, 57, 2134-2145.	1.1	197
4	Coupling of excitons and defect states in boron-nitride nanostructures. Physical Review B, 2011, 83, .	1.1	177
5	Ab initiostudy of the annealing of vacancies and interstitials in cubic SiC: Vacancy-interstitial recombination and aggregation of carbon interstitials. Physical Review B, 2004, 69, .	1.1	172
6	Divacancy in 4H-SiC. Physical Review Letters, 2006, 96, 055501.	2.9	172
7	Application of generalized gradient approximations: The diamondâ€“Î²-tin phase transition in Si and Ge. Physical Review B, 1995, 52, 2550-2556.	1.1	153
8	Identification of the Carbon Antisite-Vacancy Pair in4H-SiC. Physical Review Letters, 2006, 96, 145501.	2.9	72
9	Ab InitioMolecular Dynamics Study of the Desorption ofD2from Si(100). Physical Review Letters, 1997, 79, 701-704.	2.9	67
10	Signature of intrinsic defects in SiC:Ab initiocalculations of hyperfine tensors. Physical Review B, 2003, 67, .	1.1	66
11	Many-Body Effects in the Excitation Spectrum of a Defect in SiC. Physical Review Letters, 2010, 105, 026401.	2.9	66
12	A Dynamic Landscape from Femtoseconds to Minutes for Excess Electrons at Iceâ”Metal Interfaces. Journal of Physical Chemistry C, 2009, 113, 979-988.	1.5	61
13	Electrical Charge State Manipulation of Single Silicon Vacancies in a Silicon Carbide Quantum Optoelectronic Device. Nano Letters, 2019, 19, 7173-7180.	4.5	61
14	Ab initio description of highly correlated states in defects for realizing quantum bits. Npj Quantum Materials, 2018, 3, .	1.8	60
15	Structure and vibrational spectra of carbon clusters in SiC. Physical Review B, 2004, 70, .	1.1	50
16	Solubility of nitrogen and phosphorus in 4H-SiC: A theoretical study. Applied Physics Letters, 2004, 85, 58-60.	1.5	50
17	Spin and photophysics of carbon-antisite vacancy defect in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>4</mml:mn><mml:mi>H</mml:mi></mml:mrow></mml:math> carbide: A potential quantum bit. Physical Review B, 2015, 91, .	1.1	50
18	From White to Red: Electricâ€Field Dependent Chromaticity of Lightâ€Emitting Electrochemical Cells based on Archetypal Porphyrins. Advanced Functional Materials, 2016, 26, 6737-6750.	7.8	49

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19	Different roles of carbon and silicon interstitials in the interstitial-mediated boron diffusion inSiC. Physical Review B, 2004, 70, .	1.1	48
20	Identification of intrinsic defects in SiC: Towards an understanding of defect aggregates by combining theoretical and experimental approaches. Physica Status Solidi (B): Basic Research, 2008, 245, 1281-1297.	0.7	40
21	Boron in SiC: Structure and Kinetics. Materials Science Forum, 2001, 353-356, 447-450.	0.3	39
22	Carbon antisite clusters in SiC: A possible pathway to theDIIcenter. Physical Review B, 2004, 69, .	1.1	39
23	Self Diffusion in SiC: the Role of Intrinsic Point Defects. Materials Science Forum, 2001, 353-356, 323-326.	0.3	37
24	Orbital-Symmetry-Dependent Electron Transfer through Molecules Assembled on Metal Substrates. Journal of Physical Chemistry Letters, 2012, 3, 436-440.	2.1	35
25	Electron spectrum of epitaxial graphene monolayers. Physical Review B, 2010, 82, .	1.1	34
26	Theory of Self-Diffusion in GaAs*. Zeitschrift Fur Physikalische Chemie, 1997, 200, 195-207.	1.4	33
27	The Nature and Diffusion of Intrinsic Point Defects in SiC. Materials Science Forum, 2002, 389-393, 471-476.	0.3	26
28	Chemical termination of the CsCl-structure FeSi/Si(111) film surface and its multilayer relaxation. Physical Review B, 2003, 67, .	1.1	24
29	Ab Initio Study of Intrinsic Point defects and Dopant-defect Complexes in SiC: Application to Boron Diffusion. Materials Science Forum, 2000, 338-342, 949-952.	0.3	23
30	Interstitials in SiC: a model for the DII center. Physica B: Condensed Matter, 2001, 308-310, 656-659.	1.3	19
31	Hydroxylation Induced Alignment of Metal Oxide Nanocubes. Angewandte Chemie - International Edition, 2017, 56, 1407-1410.	7.2	19
32	Identification and Annealing of Common Intrinsic Defect Centers. Materials Science Forum, 2003, 433-436, 471-476.	0.3	15
33	Dynamical Simulation of Electron Transfer Processes in Alkanethiolate Self-Assembled Monolayers at the Au(111) Surface. Journal of Physical Chemistry C, 2013, 117, 25334-25342.	1.5	15
34	Incomplete Bilayer Termination of the Ice (0001) Surface. Journal of Physical Chemistry C, 2016, 120, 1097-1109.	1.5	15
35	Thermally stable carbon-related centers in 6H-SiC: Photoluminescence spectra and microscopic models. Physical Review B, 2006, 73, .	1.1	14
36	Vibrationally dependent electron-electron interactions in resonant electron transport through single-molecule junctions. Physical Review B, 2016, 93, .	1.1	14

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37	Deactivation of nitrogen donors in silicon carbide. Physical Review B, 2006, 74, .	1.1	13
38	Graphene on cubic and hexagonal SiC: A comparative theoretical study. Physical Review B, 2012, 86, .	1.1	12
39	Carbon Interstitials in SiC: A Model for the D_{II} Center. Materials Science Forum, 2002, 389-393, 481-484.	0.3	11
40	Ab-Initio Study of Dopant Interstitials in 4H-SiC. Materials Science Forum, 2005, 483-485, 523-526.	0.3	11
41	Publisherâ€™s Note: Divacancy in 4H-SiC [Phys. Rev. Lett.96, 055501 (2006)]. Physical Review Letters, 2006, 96, .	2.9	11
42	Divacancy and Its Identification: Theory. Materials Science Forum, 2006, 527-529, 523-526.	0.3	11
43	Microscopic Insight into Electron-Induced Dissociation of Aromatic Molecules on Ice. Physical Review Letters, 2018, 121, 206001.	2.9	10
44	Electronic structure of tetraphenylporphyrin layers on Ag(100). Physical Review B, 2017, 95, .	1.1	9
45	Diffusion of clusters down aluminum islands. Computational Materials Science, 2002, 23, 85-94.	1.4	8
46	Cobalt and Iron Ions in MgO Nanocrystals: Should They Stay or Should They Go. Journal of Physical Chemistry C, 2019, 123, 25991-26004.	1.5	8
47	Efficient self-consistent method using basis splines for the investigation of interacting two-dimensional electrons in a random impurity potential. Physical Review B, 2001, 64, .	1.1	7
48	Defect Migration and Annealing Mechanisms. Advanced Texts in Physics, 2004, , 27-55.	0.5	7
49	From Anhydrous Zinc Oxide Nanoparticle Powders to Aqueous Colloids: Impact of Water Condensation and Organic Salt Adsorption on Free Exciton Emission. Langmuir, 2019, 35, 8741-8747.	1.6	7
50	Identification of divacancies in 4H-SiC. Physica B: Condensed Matter, 2006, 376-377, 334-337.	1.3	6
51	Divacancy Model for P6/P7 Centers in 4H- and 6H-SiC. Materials Science Forum, 2006, 527-529, 527-530.	0.3	6
52	Kinetic Mechanisms for the Deactivation of Nitrogen in SiC. Materials Science Forum, 2006, 527-529, 621-624.	0.3	6
53	Effect of crystallization on the electronic and optical properties of archetypical porphyrins. Physical Chemistry Chemical Physics, 2020, 22, 3825-3830.	1.3	6
54	Impact of Electron Solvation on Ice Structures at the Molecular Scale. Journal of Physical Chemistry Letters, 2020, 11, 1310-1316.	2.1	6

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55	A Theoretical Study of Carbon Clusters in SiC: a Sink and a Source of Carbon Interstitials. Materials Science Forum, 2004, 457-460, 449-452.	0.3	5
56	Toward Functional Inorganic/Organic Hybrids: Phenoxy-allyl-PTCDI Synthesis, Experimentally and Theoretically Determined Properties of the Isolated Molecule, Layer Characteristics, and the Interface Formation of Phenoxy-allyl-PTCDI on Si(111):H Determined by SXPS and DFT. Journal of Physical Chemistry C, 2011, 115, 21139-21150.	1.5	5
57	Electroluminescence: From White to Red: Electricâ€Field Dependent Chromaticity of Lightâ€Emitting Electrochemical Cells based on Archetypal Porphyrins (Adv. Funct. Mater. 37/2016). Advanced Functional Materials, 2016, 26, 6736-6736.	7.8	5
58	Doping of 4H-SiC with Group IV Elements. Materials Science Forum, 0, 858, 301-307.	0.3	5
59	Dynamical simulation of electron transfer processes in self-assembled monolayers at metal surfaces using a density matrix approach. Journal of Chemical Physics, 2018, 148, 124705.	1.2	5
60	Self-metalation of a free-base porphyrin on a metal oxide surface mediated by extended defects: Insight from ab initio molecular dynamics simulations. Surface Science, 2022, 723, 122101.	0.8	5
61	The Solubility and Defect Equilibrium on the n-Type Dopants Nitrogen and Phosphorus in 4H-SiC: A Theoretical Study. Materials Science Forum, 2004, 457-460, 715-718.	0.3	4
62	Signature of the Negative Carbon Vacancy-Antisite Complex. Materials Science Forum, 2006, 527-529, 539-542.	0.3	4
63	Removing the orientational degeneracy of the TS defect in 4Hâ€“SiC by electric fields and strain. New Journal of Physics, 2021, 23, 073002.	1.2	4
64	Morphology dependent interaction between Co(<scp>ii</scp>)-tetraphenylporphyrin and the MgO(100) surface. Physical Chemistry Chemical Physics, 2021, 23, 2105-2116.	1.3	4
65	Point Defects and their Aggregation in Silicon Carbide. Materials Science Forum, 2007, 556-557, 439-444.	0.3	3
66	(Nitrogen-Vacancy)-Complex Formation in SiC: Experiment and Theory. Materials Science Forum, 2007, 556-557, 307-312.	0.3	3
67	Defects Identified in SiC and Their Implications. Materials Science Forum, 2008, 600-603, 285-290.	0.3	3
68	Localization phase diagram for a disordered system in a magnetic field in two dimensions. Journal of Physics Condensed Matter, 1993, 5, 6043-6054.	0.7	2
69	High Energy Local Vibrational Modes of Carbon Aggregates in SiC: Experimental and Theoretical Insight. Materials Science Forum, 2006, 527-529, 465-468.	0.3	2
70	Point Defects in SiC. Materials Research Society Symposia Proceedings, 2008, 1069, 1.	0.1	2
71	Persistent Conductivity in n-Type 3C-SiC Observed at Low Temperatures. Materials Science Forum, 2014, 778-780, 265-268.	0.3	2
72	Kinetic Aspects of the Interstitial-Mediated Boron Diffusion in SiC. Materials Science Forum, 2005, 483-485, 527-530.	0.3	0

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73	Modeling of Atomistic Processes in Semiconductors: from Defect Signatures to a Hierarchy of Annealing Mechanisms. Materials Research Society Symposia Proceedings, 2006, 978, .	0.1	0
74	Organisation von Metalloxidâ€NanowÃ¼rfeln durch Hydroxylierung. Angewandte Chemie, 2017, 129, 1428-1432.	1.6	0