Michel Bockstedte

List of Publications by Citations

74 papers	2,760 citations	26 h-index	52 g-index
75 ext. papers	2,938 ext. citations	3.5 avg, IF	4.72 L-index

#	Paper	IF	Citations
74	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	4.2	628
73	Ab initio study of the migration of intrinsic defects in 3C-SiC. *Physical Review B*, **2003**, 68,	3.3	215
72	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	3.3	174
71	Ab initio study of the annealing of vacancies and interstitials in cubic SiC: Vacancy-interstitial recombination and aggregation of carbon interstitials. *Physical Review B*, **2004**, 69,	3.3	156
70	Divacancy in 4H-SiC. *Physical Review Letters*, **2006**, 96, 055501	7.4	151
69	Coupling of excitons and defect states in boron-nitride nanostructures. *Physical Review B*, **2011**, 83,	3.3	147
68	Application of generalized gradient approximations: The diamond- beta -tin phase transition in Si and Ge. *Physical Review B*, **1995**, 52, 2550-2556	3.3	121
67	Identification of the carbon antisite-vacancy pair in 4H-SiC. *Physical Review Letters*, **2006**, 96, 145501	7.4	66
66	Ab Initio Molecular Dynamics Study of the Desorption of D2 from Si(100). *Physical Review Letters*, **1997**, 79, 701-704	7.4	65
65	Signature of intrinsic defects in SiC: Ab initio calculations of hyperfine tensors. *Physical Review B*, **2003**, 67,	3.3	61
64	Many-body effects in the excitation spectrum of a defect in SiC. *Physical Review Letters*, **2010**, 105, 026401	7.4	60
63	A Dynamic Landscape from Femtoseconds to Minutes for Excess Electrons at Ice-Metal Interfaces. *Journal of Physical Chemistry C*, **2009**, 113, 979-988	3.8	58
62	From White to Red: Electric-Field Dependent Chromaticity of Light-Emitting Electrochemical Cells based on Archetypal Porphyrins. *Advanced Functional Materials*, **2016**, 26, 6737-6750	15.6	44
61	Solubility of nitrogen and phosphorus in 4H-SiC: A theoretical study. *Applied Physics Letters*, **2004**, 85, 58-60	3.4	42
60	Spin and photophysics of carbon-antisite vacancy defect in 4H silicon carbide: A potential quantum bit. *Physical Review B*, **2015**, 91,	3.3	41
59	Structure and vibrational spectra of carbon clusters in SiC. *Physical Review B*, **2004**, 70,	3.3	41
58	Different roles of carbon and silicon interstitials in the interstitial-mediated boron diffusion in SiC. *Physical Review B*, **2004**, 70,	3.3	40

57	Ab initio description of highly correlated states in defects for realizing quantum bits. *Npj Quantum Materials*, **2018**, 3,	5	38
56	Electrical Charge State Manipulation of Single Silicon Vacancies in a Silicon Carbide Quantum Optoelectronic Device. *Nano Letters*, **2019**, 19, 7173-7180	11.5	36
55	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	1.3	35
54	Carbon antisite clusters in SiC: A possible pathway to the DII center. *Physical Review B*, **2004**, 69,	3.3	35
53	Self Diffusion in SiC: the Role of Intrinsic Point Defects. *Materials Science Forum*, **2001**, 353-356, 323-326	0.4	35
52	Orbital-Symmetry-Dependent Electron Transfer through Molecules Assembled on Metal Substrates. *Journal of Physical Chemistry Letters*, **2012**, 3, 436-40	6.4	33
51	Boron in SiC: Structure and Kinetics. *Materials Science Forum*, **2001**, 353-356, 447-450	0.4	33
50	Electron spectrum of epitaxial graphene monolayers. *Physical Review B*, **2010**, 82,	3.3	32
49	Theory of Self-Diffusion in GaAs*. *Zeitschrift Fur Physikalische Chemie*, **1997**, 200, 195-207	3.1	30
48	The Nature and Diffusion of Intrinsic Point Defects in SiC. *Materials Science Forum*, **2002**, 389-393, 471-476	0.4	26
47	Chemical termination of the CsCl-structure FeSi/Si(111) film surface and its multilayer relaxation. *Physical Review B*, **2003**, 67,	3.3	24
46	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	0.4	21
45	Interstitials in SiC: a model for the DII center. *Physica B: Condensed Matter*, **2001**, 308-310, 656-659	2.8	16
44	Incomplete Bilayer Termination of the Ice (0001) Surface. *Journal of Physical Chemistry C*, **2016**, 120, 1097-1109	3.8	14
43	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	3.8	14
42	Deactivation of nitrogen donors in silicon carbide. *Physical Review B*, **2006**, 74,	3.3	13
41	Hydroxylation Induced Alignment of Metal Oxide Nanocubes. *Angewandte Chemie - International Edition*, **2017**, 56, 1407-1410	16.4	12
40	Vibrationally dependent electron-electron interactions in resonant electron transport through single-molecule junctions. *Physical Review B*, **2016**, 93,	3.3	12

39	Identification and Annealing of Common Intrinsic Defect Centers. *Materials Science Forum*, **2003**, 433-436, 471-476	0.4	12
38	Graphene on cubic and hexagonal SiC: A comparative theoretical study. *Physical Review B*, **2012**, 86,	3.3	11
37	Thermally stable carbon-related centers in 6H-SiC: Photoluminescence spectra and microscopic models. *Physical Review B*, **2006**, 73,	3.3	11
36	Carbon Interstitials in SiC: A Model for the DII Center. *Materials Science Forum*, **2002**, 389-393, 481-484	0.4	11
35	Divacancy and Its Identification: Theory. *Materials Science Forum*, **2006**, 527-529, 523-526	0.4	10
34	Publisher Note: Divacancy in 4H-SiC [Phys. Rev. Lett. 96, 055501 (2006)]. *Physical Review Letters*, **2006**, 96,	7.4	10
33	Ab-Initio Study of Dopant Interstitials in 4H-SiC. *Materials Science Forum*, **2005**, 483-485, 523-526	0.4	9
32	Diffusion of clusters down aluminum islands. *Computational Materials Science*, **2002**, 23, 85-94	3.2	8
31	Electronic structure of tetraphenylporphyrin layers on Ag(100). *Physical Review B*, **2017**, 95,	3.3	7
30	Cobalt and Iron Ions in MgO Nanocrystals: Should They Stay or Should They Go. *Journal of Physical Chemistry C*, **2019**, 123, 25991-26004	3.8	7
29	Defect Migration and Annealing Mechanisms. *Advanced Texts in Physics*, **2004**, 27-55		7
28	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,	3.3	7
27	Microscopic Insight into Electron-Induced Dissociation of Aromatic Molecules on Ice. *Physical Review Letters*, **2018**, 121, 206001	7.4	7
26	Divacancy Model for P6/P7 Centers in 4H- and 6H-SiC. *Materials Science Forum*, **2006**, 527-529, 527-530	0.4	6
25	Kinetic Mechanisms for the Deactivation of Nitrogen in SiC. *Materials Science Forum*, **2006**, 527-529, 621-624	0.4	6
24	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	4	5
23	Doping of 4H-SiC with Group IV Elements. *Materials Science Forum*, **2016**, 858, 301-307	0.4	5
22	A Theoretical Study of Carbon Clusters in SiC: a Sink and a Source of Carbon Interstitials. *Materials Science Forum*, **2004**, 457-460, 449-452	0.4	5

21	Impact of Electron Solvation on Ice Structures at the Molecular Scale. *Journal of Physical Chemistry Letters*, **2020**, 11, 1310-1316	6.4	4
20	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	3.9	4
19	Identification of divacancies in 4H-SiC. *Physica B: Condensed Matter*, **2006**, 376-377, 334-337	2.8	4
18	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	0.4	4
17	Effect of crystallization on the electronic and optical properties of archetypical porphyrins. *Physical Chemistry Chemical Physics*, **2020**, 22, 3825-3830	3.6	3
16	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	3.8	3
15	Defects Identified in SiC and Their Implications. *Materials Science Forum*, **2008**, 600-603, 285-290	0.4	3
14	Signature of the Negative Carbon Vacancy-Antisite Complex. *Materials Science Forum*, **2006**, 527-529, 539-542	0.4	3
13	Electroluminescence: From White to Red: Electric-Field Dependent Chromaticity of Light-Emitting Electrochemical Cells based on Archetypal Porphyrins (Adv. Funct. Mater. 37/2016). *Advanced Functional Materials*, **2016**, 26, 6736-6736	15.6	3
12	Morphology dependent interaction between Co(II)-tetraphenylporphyrin and the MgO(100) surface. *Physical Chemistry Chemical Physics*, **2021**, 23, 2105-2116	3.6	3
11	Persistent Conductivity in n-Type 3C-SiC Observed at Low Temperatures. *Materials Science Forum*, **2014**, 778-780, 265-268	0.4	2
10	Point Defects in SiC. *Materials Research Society Symposia Proceedings*, **2008**, 1069, 1		2
9	High Energy Local Vibrational Modes of Carbon Aggregates in SiC: Experimental and Theoretical Insight. *Materials Science Forum*, **2006**, 527-529, 465-468	0.4	2
8	Point Defects and their Aggregation in Silicon Carbide. *Materials Science Forum*, **2007**, 556-557, 439-444	0.4	2
7	(Nitrogen-Vacancy)-Complex Formation in SiC: Experiment and Theory. *Materials Science Forum*, **2007**, 556-557, 307-312	0.4	2
6	Localization phase diagram for a disordered system in a magnetic field in two dimensions. *Journal of Physics Condensed Matter*, **1993**, 5, 6043-6054	1.8	2
5	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**, 122101	1.8	1
4	Organisation von Metalloxid-Nanowürfeln durch Hydroxylierung. *Angewandte Chemie*, **2017**, 129, 1428-1432	3.6	

3	Kinetic Aspects of the Interstitial-Mediated Boron Diffusion in SiC. *Materials Science Forum*, **2005**, 483-485, 527-530	0.4
2	Identification of Intrinsic Defects in SiC: Towards an Understanding of Defect Aggregates by Combining Theoretical and Experimental Approaches115-145	
1	Removing the orientational degeneracy of the TS defect in 4H-SiC by electric fields and strain. *New Journal of Physics*, **2021**, 23, 073002	2.9