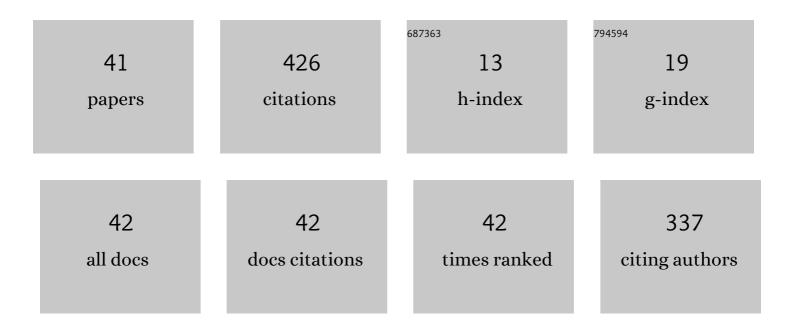


## List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Modeling arsenic deactivation through arsenic-vacancy clusters using an atomistic kinetic Monte Carlo approach. Applied Physics Letters, 2005, 86, 252103.	3.3	31
2	Optical admittance spectroscopy: A new method for deep level characterization. Journal of Applied Physics, 1987, 61, 2541-2545.	2.5	29
3	Physical atomistic kinetic Monte Carlo modeling of Fermi-level effects of species diffusing in silicon. Physical Review B, 2005, 72, .	3.2	27
4	Physical modeling and implementation scheme of native defect diffusion and interdiffusion in SiGe heterostructures for atomistic process simulation. Journal of Applied Physics, 2011, 109, .	2.5	27
5	Sulfur Hydrogen Bonding in Isolated Monohydrates: Furfuryl Mercaptan versus Furfuryl Alcohol. Chemistry - A European Journal, 2018, 24, 6564-6571.	3.3	27
6	Atomistic Monte Carlo simulations of three-dimensional polycrystalline thin films. Journal of Applied Physics, 2003, 94, 163-168.	2.5	23
7	Ion-beam amorphization of semiconductors: A physical model based on the amorphous pocket population. Journal of Applied Physics, 2005, 98, 046104.	2.5	21
8	Sulfur hydrogen bonding and internal dynamics in the monohydrates of thenyl mercaptan and thenyl alcohol. Physical Chemistry Chemical Physics, 2020, 22, 12412-12421.	2.8	21
9	An improved molecular dynamics scheme for ion bombardment simulations. Nuclear Instruments & Methods in Physics Research B, 1995, 102, 7-11.	1.4	20
10	Modeling charged defects, dopant diffusion and activation mechanisms for TCAD simulations using kinetic Monte Carlo. Nuclear Instruments & Methods in Physics Research B, 2006, 253, 63-67.	1.4	19
11	Comprehensive model of damage accumulation in silicon. Journal of Applied Physics, 2008, 103, .	2.5	16
12	Physically based modelling of damage, amorphization, and recrystallization for predictive device-size process simulation. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2004, 114-115, 151-155.	3.5	14
13	Dose effects on amorphous silicon sputtering by argon ions: A molecular dynamics simulation. Journal of Applied Physics, 1997, 81, 1488-1494.	2.5	13
14	An Efficient Microkinetic Modeling Protocol: Start with Only the Dominant Mechanisms, Adjust All Parameters, and Build the Complete Model Incrementally. ACS Catalysis, 2019, 9, 4804-4809.	11.2	13
15	Inâ€Diffusion and Annealing Kinetics of Palladium in Silicon. Journal of the Electrochemical Society, 1993, 140, 868-870.	2.9	12
16	Fermi-level effects in semiconductor processing: A modeling scheme for atomistic kinetic Monte Carlo simulators. Journal of Applied Physics, 2005, 98, 053709.	2.5	12
17	A DFT-Based Computational-Experimental Methodology for Synthetic Chemistry: Example of Application to the Catalytic Opening of Epoxides by Titanocene. Journal of Organic Chemistry, 2017, 82, 3760-3766.	3.2	12
18	Molecular Recognition, Transient Chirality and Sulfur Hydrogen Bonding in the Benzyl Mercaptan Dimer. Symmetry, 2021, 13, 2022.	2.2	11

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19	Kinetic Monte Carlo simulations: an accurate bridge between ab initio calculations and standard process experimental data. Materials Science in Semiconductor Processing, 2000, 3, 59-63.	4.0	9
20	Physically based modeling of dislocation loops in ion implantation processing in silicon. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2005, 124-125, 404-408.	3.5	7
21	Ion implant simulations: Kinetic Monte Carlo annealing assessment of the dominant features. Applied Physics Letters, 2004, 84, 4962-4964.	3.3	6
22	Physical modeling of Fermi-level effects for decanano device process simulations. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2004, 114-115, 284-289.	3.5	6
23	Dose loss and segregation of boron and arsenic at the Si/SiO2 interface by atomistic kinetic Monte Carlo simulations. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2005, 124-125, 392-396.	3.5	6
24	Atomistic modeling of defect diffusion and interdiffusion in SiGe heterostructures. Thin Solid Films, 2010, 518, 2448-2453.	1.8	6
25	Computer simulation of point-defect distributions generated by ion implantation. Nuclear Instruments & Methods in Physics Research B, 1993, 80-81, 172-175.	1.4	5
26	Comprehensive, physically based modelling of As in Si. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2004, 114-115, 135-140.	3.5	5
27	Constant-capacitance deep-level optical spectroscopy. Solid-State Electronics, 1989, 32, 287-293.	1.4	4
28	Detailed computer simulation of ion implantation processes into crystals. Materials Science and Technology, 1995, 11, 1191-1193.	1.6	4
29	Comprehensive modeling of ion-implant amorphization in silicon. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2005, 124-125, 383-385.	3.5	4
30	Rotational spectra of tetracyclic quinolizidine alkaloids: does a water molecule flip sparteine?. Physical Chemistry Chemical Physics, 2017, 19, 17553-17559.	2.8	4
31	Monte Carlo Atomistic Simulation of Polycrystalline Aluminum Deposition. Materials Research Society Symposia Proceedings, 1998, 514, 127.	0.1	3
32	Optical capture cross sections of palladium in silicon. Journal of Applied Physics, 1991, 69, 298-301.	2.5	2
33	A kinetic Monte Carlo annealing assessment of the dominant features from ion implant simulations. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2004, 114-115, 345-348.	3.5	2
34	15-Hydroxygermacranolides as Sources of Structural Diversity: Synthesis of Sesquiterpene Lactones by Cyclization and Rearrangement Reactions. Experimental and DFT Study. Journal of Organic Chemistry, 2018, 83, 5480-5495.	3.2	2
35	Molecular dynamics simulations of ion bombardment processes. Materials Science and Technology, 1997, 13, 893-896.	1.6	1
36	Chirality-Puckering correlation and intermolecular interactions in Sphingosines: Rotational spectroscopy of jaspine B3 and its monohydrate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 267, 120531.	3.9	1

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37	<i>Cis</i> and <i>trans</i> platinum( <scp>ii</scp> ) N-heterocyclic carbene isomers: synthesis, characterization and biological activity. New Journal of Chemistry, 2022, 46, 14221-14226.	2.8	1
38	Bimodal distribution of damage morphology generated by ion implantation. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2005, 124-125, 389-391.	3.5	0
39	Ion-implant simulations: The effect of defect spatial correlation on damage accumulation. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2005, 124-125, 386-388.	3.5	Ο
40	Current Capabilities and Future Prospects of Atomistic Process Simulation. , 2007, , .		0
41	Rotational spectroscopy of organophosphorous chemical agents: cresyl and phenyl saligenin phosphates. Physical Chemistry Chemical Physics, 2019, 21, 16418-16422.	2.8	0