Layla Martin-Samos

List of Publications by Year
in descending order

69 papers	19,977 citations	331670 21 h-index	149698 56 g-index
71 all docs	71 docs citations	71 times ranked	22987 citing authors

#	Article	IF	Citations
1	Common defects in diamond lattices as instances of the general T <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mo>âŠ—</mml:mo></mml:math> <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>(</mml:mo><mml:mi>e</mml:mi><mml:mo>+</mml:mo> Jahn-Teller effect. Physical Review Materials, 2022, 6, .	2.4	1
2	Iterative Rotations and Assignments (IRA): A shape matching algorithm for atomic structures. Software Impacts, 2022, 12, 100264.	1.4	2
3	O2 Loaded Germanosilicate Optical Fibers: Experimental In Situ Investigation and Ab Initio Simulation Study of GLPC Evolution under Irradiation. Applied Sciences (Switzerland), 2022, 12, 3916.	2.5	0
4	Activationâ€“Relaxation Technique: An efficient way to find minima and saddle points of potential energy surfaces. Computational Materials Science, 2022, 209, 111363.	3.0	5
5	Paramagnetic Intrinsic Point Defects in Alkali Phosphate Glasses: Unraveling the P₃ Center Origin and Local Environment Effects. Journal of Physical Chemistry C, 2021, 125, 8741-8751.	3.1	1
6	IRA: A Shape Matching Approach for Recognition and Comparison of Generic Atomic Patterns. Journal of Chemical Information and Modeling, 2021, 61, 5446-5457.	5.4	3
7	Kinetic Monte Carlo for Process Simulation: First Principles Calibrated Parameters for BO2. , 2021, , .		0
8	Developing a Neural Network potential to investigate interface phenomena in solid-phase epitaxy. , 2021, , .		0
9	Collective dipole effects in ionic transport under electric fields. Nature Communications, 2020, 11, 3330.	12.8	6
10	Finding Reaction Pathways and Transition States: r-ARTn and d-ARTn as an Efficient and Versatile Alternative to String Approaches. Journal of Chemical Theory and Computation, 2020, 16, 6726-6734.	5.3	21
11	A comprehensive theoretical picture of E centers in silicon: From optical properties to vacancy-mediated dopant diffusion. Journal of Applied Physics, 2020, 127, 085703.	2.5	8
12	First-principles characterization of Mg low-index surfaces: Structure, reconstructions, and surface core-level shifts. Physical Review B, 2019, 100, .	3.2	1
13	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	19.0	655
14	Vibrational and structural properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">P</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:math> glass: Advances from a combined modeling approach. Physical Review B, 2019, 100, .	3.2	7
15	Electronic and structural properties of interstitial titanium in crystalline silicon from first-principles simulations. , 2019, , .		0
16	First-Principles Investigation of Paramagnetic Centers in P2 O5 Based Glasses. , 2019, , .		0
17	Defect creation and Diffusion under electric fields from first-principles: the prototypical case of silicon dioxide. , 2019, , .		1
18	Study of silica-based intrinsically emitting nanoparticles produced by an excimer laser. Beilstein Journal of Nanotechnology, 2019, 10, 211-221.	2.8	1

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19	v-P2O5 micro-clustering in P-doped silica studied by a first-principles Raman investigation. Scientific Reports, 2019, 9, 7126.	3.3	7
20	Overview of radiation induced point defects in silica-based optical fibers. Reviews in Physics, 2019, 4, 100032.	8.9	208
21	Optical Properties of Saturated and Unsaturated Carbonyl Defects in Polyethylene. Journal of Physical Chemistry B, 2018, 122, 2023-2030.	2.6	5
22	Simulation of Single-Particle Displacement Damage in Siliconâ€"Part III: First Principle Characterization of Defect Properties. IEEE Transactions on Nuclear Science, 2018, 65, 724-731.	2.0	16
23	Ni-Ion and $gamma$ -Ray Irradiated Silica-Based Glasses Characterized by Luminescence and Raman Spectroscopies. IEEE Transactions on Nuclear Science, 2018, 65, 1604-1611.	2.0	0
24	Optical absorption spectra of P defects in vitreous silica. Optical Materials Express, 2018, 8, 385.	3.0	9
25	Correlations between Structural and Optical Properties of Peroxy Bridges from First Principles. Journal of Physical Chemistry C, 2017, 121, 4002-4010.	3.1	9
26	Study of point defects in as-drawn and irradiated Ge-doped optical fibers using cathodoluminescence. IOP Conference Series: Materials Science and Engineering, 2017, 169, 012006.	0.6	1
27	Irradiation temperature effects on the induced point defects in Ge-doped optical fibers.. IOP Conference Series: Materials Science and Engineering, 2017, 169, 012008.	0.6	0
28	Coupled irradiation-temperature effects on induced point defects in germanosilicate optical fibers. Journal of Materials Science, 2017, 52, 10697-10708.	3.7	3
29	Photoactivated processes in optical fibers: generation and conversion mechanisms of twofold coordinated Si and Ge atoms. Nanotechnology, 2017, 28, 195202.	2.6	15
30	Evidence of enhanced photocurrent response in corannulene films. RSC Advances, 2017, 7, 45601-45606.	3.6	5
31	Effect of irradiation temperature on the radiation induced attenuation of Ge-doped fibers. , 2016, , .		1
32	Ge-doped silica nanoparticles: production and characterisation. Optical Materials Express, 2016, 6, 2213.	3.0	4
33	Cathodoluminescence Characterization of Point Defects in Optical Fibers. IEEE Transactions on Nuclear Science, 2016, , 1-1.	2.0	6
34	Cathodoluminescence investigation of Ge-point defects in silica-based optical fibers. Journal of Luminescence, 2016, 179, 1-7.	3.1	7
35	Irradiation temperature influence on the in-situ measured radiation induced attenuation of Ge-doped fibers. IEEE Transactions on Nuclear Science, 2016, , 1-1.	2.0	3
36	Investigation of point defects in silica-based optical fibers by cathodoluminescence. , 2016, , .		0

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37	Gamma and x-ray irradiation effects on different Ge and Ge/F doped optical fibers. Journal of Applied Physics, 2015, 118, .	2.5	17
38	QMMMW: A wrapper for QM/MM simulations with Quantum ESPRESSO Âand LAMMPS. Computer Physics Communications, 2015, 195, 191-198.	7.5	6
39	Buckybowl superatom states: a unique route for electron transport?. Physical Chemistry Chemical Physics, 2015, 17, 6114-6121.	2.8	23
40	Paramagnetic centers in amorphous GeO2. Microelectronic Engineering, 2015, 147, 130-133.	2.4	3
41	Ge(2), Ge(1) and Ge-Eâ€² centers in irradiated Ge-doped silica: a first-principles EPR study. Optical Materials Express, 2015, 5, 1054.	3.0	29
42	EPR parameters of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mi>E</mml:mi><mml:mo>â€²</mml:mo></mml:msup></mm in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>v</mml:mi><mml:mo>â”</mml:mo><mml:msub><mml:mrow><mml:m mathvariant="normal">SiO</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math>from first-principles calculations. Physical Review B, 2014, 90, .	3.2	26
43	Structureâ€“Property Relationships of Curved Aromatic Materials from First Principles. Accounts of Chemical Research, 2014, 47, 3310-3320.	15.6	27
44	Neutron Irradiation Effects on the Structural Properties of KU1, KS-4V and I301 Silica Glasses. IEEE Transactions on Nuclear Science, 2014, 61, 1522-1530.	2.0	21
45	Coupled Theoretical and Experimental Studies for the Radiation Hardening of Silica-Based Optical Fibers. IEEE Transactions on Nuclear Science, 2014, 61, 1819-1825.	2.0	23
46	Oxygen deficient centers in silica: optical properties within many-body perturbation theory. Journal of Physics Condensed Matter, 2013, 25, 335502.	1.8	22
47	Enhancement of DFT-calculations at petascale: Nuclear Magnetic Resonance, Hybrid Density Functional Theory and Carâ€“Parrinello calculations. Computer Physics Communications, 2013, 184, 1827-1833.	7.5	33
48	Coupled theoretical and experimental studies for the radiation hardening of silica-based optical fibers. , 2013, , .		1
49	Neutron irradiation effects on the structural properties of KU1, KS-4V and I301 silica glasses. , 2013, , .		0
50	Ab initiocomplex band structure of conjugated polymers: Effects of hydrid density functional theory and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="italic">GW</mml:mi></mml:mrow></mml:math>schemes. Physical Review B, 2012, 85, .	3.2	34
51	Effect of Molecular Packing on Corannulene-Based Materials Electroluminescence. Journal of the American Chemical Society, 2011, 133, 14002-14009.	13.7	77
52	First principles study of oxygen-deficient centers in pure and Ge-doped silica. Journal of Non-Crystalline Solids, 2011, 357, 1994-1999.	3.1	19
53	SiO₂ in density functional theory and beyond. Physica Status Solidi (B): Basic Research, 2011, 248, 1061-1066.	1.5	15
54	Unraveling effects of disorder on the electronic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu first principles. Physical Review B, 2010, 81, .	3.2	22

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55	Charged Oxygen Defects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>SiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>: Going beyond Local and Semilocal Approximations to Density Functional Theory. Physical Review Letters, 2010, 104, 075502.	7.8	31
56	Optical properties of silicon nanocrystallites in SiO2 matrix: Crystalline vs. amorphous case. Superlattices and Microstructures, 2009, 46, 246-252.	3.1	20
57	SaX: An open source package for electronic-structure and optical-properties calculations in the GW approximation. Computer Physics Communications, 2009, 180, 1416-1425.	7.5	38
58	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502.	1.8	18,183
59	Silicon nanocrystallites in a<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> matrix: Role of disorder and size. Physical Review B, 2009, 79, .	3.2	57
60	Atomic and electronic structure of the nonpolar<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>GaN</mml:mtext><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mn>1</mml:mn></mml:mrow>	3.2	65
61	Physical Review B, 2009, 80, . Radiation Effects on Silica-Based Preforms and Optical Fibers-II: Coupling Ab initio Simulations and Experiments. IEEE Transactions on Nuclear Science, 2008, 55, 3508-3514.	2.0	32
62	Defects in amorphous<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Si</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>: Valence alternation pair model. Physical Review B, 2007, 76, .	3.2	14
63	Ab initio molecular dynamics simulations of oxygen-deficient centers in pure and Ge-doped silica glasses: Structure and optical properties. Journal of Non-Crystalline Solids, 2006, 352, 2596-2600.	3.1	10
64	Aspects of point defects energetics and diffusion in SiO2 from first principles simulations. Nuclear Instruments & Methods in Physics Research B, 2006, 250, 54-56.	1.4	6
65	Oxygen and Silicon Self-Diffusion in Quartz and Silica: The Contribution of First Principles Calculations. Defect and Diffusion Forum, 2006, 258-260, 542-553.	0.4	2
66	Oxygen Self-Diffusion Mechanisms in Silica by First-Principles. Defect and Diffusion Forum, 2005, 237-240, 115-120.	0.4	0
67	Neutral self-defects in a silica model: A first-principles study. Physical Review B, 2005, 71, .	3.2	55
68	First principle study of neutral and charged self-defects in amorphous SiO2. Journal of Non-Crystalline Solids, 2005, 351, 1825-1829.	3.1	36
69	Oxygen neutral defects in silica: Origin of the distribution of the formation energies. Europhysics Letters, 2004, 66, 680-686.	2.0	19