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	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
2	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	19.0	655
3	Overview of radiation induced point defects in silica-based optical fibers. Reviews in Physics, 2019, 4, 100032.	8.9	208
4	Effect of Molecular Packing on Corannulene-Based Materials Electroluminescence. Journal of the American Chemical Society, 2011, 133, 14002-14009.	13.7	77
5	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> Physical Review B, 2009, 80, .	3.2	65
6	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:msu Role of disorder and size. Physical Review B, 2009, 79, .	3.2	57
7	Neutral self-defects in a silica model: A first-principles study. Physical Review B, 2005, 71, .	3.2	55
8	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
9	First principle study of neutral and charged self-defects in amorphous SiO2. Journal of Non-Crystalline Solids, 2005, 351, 1825-1829.	3.1	36
10	<i>Ab initio</i>complex 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
11	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
12	Radiation Effects on Silica-Based Preforms and Optical Fibers-II: Coupling <i>Ab initio</i> Simulations and Experiments. IEEE Transactions on Nuclear Science, 2008, 55, 3508-3514.	2.0	32
13	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
14	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
15	Structureâ€“Property Relationships of Curved Aromatic Materials from First Principles. Accounts of Chemical Research, 2014, 47, 3310-3320.	15.6	27
16	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>âˆ’</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
17	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
18	Buckybowl superatom states: a unique route for electron transport?. Physical Chemistry Chemical Physics, 2015, 17, 6114-6121.	2.8	23

#	Article	IF	Citations
19	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:msub></mml:mrow></mml:math> first principles. Physical Review B, 2010, 81, .	3.2	22
20	Oxygen deficient centers in silica: optical properties within many-body perturbation theory. Journal of Physics Condensed Matter, 2013, 25, 335502.	1.8	22
21	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
22	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
23	Optical properties of silicon nanocrystallites in SiO2 matrix: Crystalline vs. amorphous case. Superlattices and Microstructures, 2009, 46, 246-252.	3.1	20
24	Oxygen neutral defects in silica: Origin of the distribution of the formation energies. Europhysics Letters, 2004, 66, 680-686.	2.0	19
25	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
26	Gamma and x-ray irradiation effects on different Ge and Ge/F doped optical fibers. Journal of Applied Physics, 2015, 118, .	2.5	17
27	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
28	SiO₂ in density functional theory and beyond. Physica Status Solidi (B): Basic Research, 2011, 248, 1061-1066.	1.5	15
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	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
31	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
32	Correlations between Structural and Optical Properties of Peroxy Bridges from First Principles. Journal of Physical Chemistry C, 2017, 121, 4002-4010.	3.1	9
33	Optical absorption spectra of P defects in vitreous silica. Optical Materials Express, 2018, 8, 385.	3.0	9
34	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
35	Cathodoluminescence investigation of Ge-point defects in silica-based optical fibers. Journal of Luminescence, 2016, 179, 1-7.	3.1	7
36	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

#	Article	IF	Citations
37	v-P2O5 micro-clustering in P-doped silica studied by a first-principles Raman investigation. Scientific Reports, 2019, 9, 7126.	3.3	7
38	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
39	QMMMW: A wrapper for QM/MM simulations with Quantum ESPRESSO Âand LAMMPS. Computer Physics Communications, 2015, 195, 191-198.	7.5	6
40	Cathodoluminescence Characterization of Point Defects in Optical Fibers. IEEE Transactions on Nuclear Science, 2016, , 1-1.	2.0	6
41	Collective dipole effects in ionic transport under electric fields. Nature Communications, 2020, 11, 3330.	12.8	6
42	Evidence of enhanced photocurrent response in corannulene films. RSC Advances, 2017, 7, 45601-45606.	3.6	5
43	Optical Properties of Saturated and Unsaturated Carbonyl Defects in Polyethylene. Journal of Physical Chemistry B, 2018, 122, 2023-2030.	2.6	5
44	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
45	Ge-doped silica nanoparticles: production and characterisation. Optical Materials Express, 2016, 6, 2213.	3.0	4
46	Paramagnetic centers in amorphous GeO2. Microelectronic Engineering, 2015, 147, 130-133.	2.4	3
47	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
48	Coupled irradiation-temperature effects on induced point defects in germanosilicate optical fibers. Journal of Materials Science, 2017, 52, 10697-10708.	3.7	3
49	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
50	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
51	Iterative Rotations and Assignments (IRA): A shape matching algorithm for atomic structures. Software Impacts, 2022, 12, 100264.	1.4	2
52	Coupled theoretical and experimental studies for the radiation hardening of silica-based optical fibers. , 2013, , .		1
53	Effect of irradiation temperature on the radiation induced attenuation of Ge-doped fibers. , 2016, , .		1
54	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

#	Article	IF	Citations
55	First-principles characterization of Mg low-index surfaces: Structure, reconstructions, and surface core-level shifts. Physical Review B, 2019, 100, .	3.2	1
56	Defect creation and Diffusion under electric fields from first-principles: the prototypical case of silicon dioxide. , 2019, , .		1
57	Study of silica-based intrinsically emitting nanoparticles produced by an excimer laser. Beilstein Journal of Nanotechnology, 2019, 10, 211-221.	2.8	1
58	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
59	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
60	Oxygen Self-Diffusion Mechanisms in Silica by First-Principles. Defect and Diffusion Forum, 2005, 237-240, 115-120.	0.4	0
61	Neutron irradiation effects on the structural properties of KU1, KS-4V and I301 silica glasses. , 2013, , .		0
62	Investigation of point defects in silica-based optical fibers by cathodoluminescence. , 2016, , .		0
63	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
64	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
65	Electronic and structural properties of interstitial titanium in crystalline silicon from first-principles simulations. , 2019, , .		0
66	First-Principles Investigation of Paramagnetic Centers in P2 O5 Based Glasses. , 2019, , .		0
67	Kinetic Monte Carlo for Process Simulation: First Principles Calibrated Parameters for BO2. , 2021, , .		0
68	Developing a Neural Network potential to investigate interface phenomena in solid-phase epitaxy. , 2021, , .		0
69	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