## Vincenzo Lordi

## List of Publications by Citations

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#	Paper	IF	Citations
87	Method for Supporting Platinum on Single-Walled Carbon Nanotubes for a Selective Hydrogenation Catalyst. <i>Chemistry of Materials</i> , <b>2001</b> , 13, 733-737	9.6	409
86	Young modulus of single-walled carbon nanotubes. <i>Journal of Applied Physics</i> , <b>1998</b> , 84, 1939-1943	2.5	306
85	Molecular mechanics of binding in carbon-nanotube polymer composites. <i>Journal of Materials Research</i> , <b>2000</b> , 15, 2770-2779	2.5	300
84	Computational and Photoelectrochemical Study of Hydrogenated Bismuth Vanadate. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 10957-10964	3.8	185
83	Lithium ion solvation and diffusion in bulk organic electrolytes from first-principles and classical reactive molecular dynamics. <i>Journal of Physical Chemistry B</i> , <b>2015</b> , 119, 1535-45	3.4	123
82	Atomistic design of thermoelectric properties of silicon nanowires. <i>Nano Letters</i> , <b>2008</b> , 8, 1111-4	11.5	116
81	Nearest-neighbor configuration in (Galn)(NAs) probed by x-ray absorption spectroscopy. <i>Physical Review Letters</i> , <b>2003</b> , 90, 145505	7.4	112
80	Structure and Oxidation Patterns of Carbon Nanotubes. <i>Journal of Materials Research</i> , <b>1998</b> , 13, 2432-2	243.7	102
79	Solvation and Dynamics of Sodium and Potassium in Ethylene Carbonate from ab Initio Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 21913-21920	3.8	99
78	. IEEE Journal of Quantum Electronics, <b>2004</b> , 40, 656-664	2	68
77	Radial compression and controlled cutting of carbon nanotubes. <i>Journal of Chemical Physics</i> , <b>1998</b> , 109, 2509-2512	3.9	57
76	Electrical properties of point defects in CdS and ZnS. <i>Applied Physics Letters</i> , <b>2013</b> , 103, 102103	3.4	51
75	Development of GaInNAsSb alloys: Growth, band structure, optical properties and applications. <i>Physica Status Solidi (B): Basic Research</i> , <b>2007</b> , 244, 2707-2729	1.3	51
74	Intrinsic point defects in aluminum antimonide. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	39
73	Charge carrier scattering by defects in semiconductors. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	37
72	Incident wavelength and polarization dependence of spectral shifts in EGaO UV photoluminescence. <i>Scientific Reports</i> , <b>2018</b> , 8, 18075	4.9	34
71	Anomalous diffusion along metal/ceramic interfaces. <i>Nature Communications</i> , <b>2018</b> , 9, 5251	17.4	33

## (2009-2005)

70	Nearest-neighbor distributions in Ga1\(\mathbb{I}\)InxNyAs1\(\mathbb{I}\) and Ga1\(\mathbb{I}\)InxNyAs1\(\mathbb{I}\)ISbz thin films upon annealing. Physical Review B, <b>2005</b> , 71,	3.3	32	
69	Electron correlation and relativity of the 5f electrons in the UZr alloy system. <i>Journal of Nuclear Materials</i> , <b>2014</b> , 444, 356-358	3.3	29	
68	Point defects in Cd(Zn)Te and TlBr: Theory. Journal of Crystal Growth, 2013, 379, 84-92	1.6	28	
67	Prospects for n-type doping of (AlxGa1⊠)2O3 alloys. <i>Applied Physics Letters</i> , <b>2020</b> , 116, 172104	3.4	26	
66	Electronic structure and defect properties of B6O from hybrid functional and many-body perturbation theory calculations: A possible ambipolar transparent conductor. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	25	
65	Ground-state properties of rare-earth metals: an evaluation of density-functional theory. <i>Journal of Physics Condensed Matter</i> , <b>2014</b> , 26, 416001	1.8	25	
64	Identification of the local sources of paramagnetic noise in superconducting qubit devices fabricated on PAl2O3 substrates using density-functional calculations. <i>Physical Review Letters</i> , <b>2014</b> , 112, 017001	7.4	24	
63	Intermixing at the absorber-buffer layer interface in thin-film solar cells: The electronic effects of point defects in Cu(In,Ga)(Se,S)2 and Cu2ZnSn(Se,S)4 devices. <i>Journal of Applied Physics</i> , <b>2014</b> , 116, 063	3505	24	
62	Carbon nanotube caps as springs: Molecular dynamics simulations. <i>Physical Review B</i> , <b>1998</b> , 58, 12649-	1265/1	24	
61	A comparison of point defects in Cd1\(\mathbb{Z}\)TxTe1\(\mathbb{J}\)Sey crystals grown by Bridgman and traveling heater methods. Journal of Applied Physics, 2017, 121, 125705	2.5	23	
60	Ab initio guided optimization of GaTe for radiation detection applications. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	22	
59	Ionic current and polarization effect in TlBr. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	21	
58	Extrinsic point defects in aluminum antimonide. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	21	
57	Quantum-confined Stark effect of GaInNAs(Sb) quantum wells at 1300🛮 600nm. <i>Applied Physics Letters</i> , <b>2004</b> , 85, 902-904	3.4	21	
56	Thermodynamics of SmCo5 compound doped with Fe and Ni: An ab initio study. <i>Journal of Alloys and Compounds</i> , <b>2018</b> , 765, 659-663	5.7	21	
55	Descriptor-Based Approach for the Prediction of Cation Vacancy Formation Energies and Transition Levels. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 5059-5063	6.4	17	
54	TopoMS: Comprehensive topological exploration for molecular and condensed-matter systems. Journal of Computational Chemistry, <b>2018</b> , 39, 936-952	3.5	16	
53	Neutron detection with single crystal organic scintillators <b>2009</b> ,		16	

52	Cd doping at PVD-CdS/CuInGaSe2 heterojunctions. Solar Energy Materials and Solar Cells, 2017, 164, 12	86144	15
51	Microstructural and Chemical Investigation of PVD-CdS/PVD- \$hbox{CuIn}_{hbox{1-x}} {hbox{Ga}}_{hbox{x}} {hbox{Se}}_{hbox{2}}\$ Heterojunctions: A Transmission Electron Microscopy Study. <i>IEEE Journal of Photovoltaics</i> , <b>2014</b> , 4, 1625-1629	3.7	15
50	Effects of growth temperature on the structural and optical properties of 1.55th GaInNAsSb quantum wells grown on GaAs. <i>Applied Physics Letters</i> , <b>2005</b> , 87, 021908	3.4	15
49	First principles calculations of point defect diffusion in CdS buffer layers: Implications for Cu(In,Ga)(Se,S)2 and Cu2ZnSn(Se,S)4-based thin-film photovoltaics. <i>Journal of Applied Physics</i> , <b>2016</b> , 119, 025703	2.5	15
48	Complex Ion Dynamics in Carbonate Lithium-Ion Battery Electrolytes. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 6589-6595	3.8	14
47	Green emission from InP-GaP quantum-dot light-emitting diodes. <i>IEEE Photonics Technology Letters</i> , <b>2006</b> , 18, 895-897	2.2	14
46	First-principles study of atomic and electronic structures of 60? perfect and 30?/90? partial glide dislocations in CdTe. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	13
45	Structural changes on annealing of MBE grown (Ga, In)(N, As) as measured by X-ray absorption fine structure. <i>Journal of Crystal Growth</i> , <b>2003</b> , 251, 408-411	1.6	13
44	Perfect Strain Relaxation in Metamorphic Epitaxial Aluminum on Silicon through Primary and Secondary Interface Misfit Dislocation Arrays. <i>ACS Nano</i> , <b>2018</b> , 12, 6843-6850	16.7	12
43	Electric-field noise from thermally activated fluctuators in a surface ion trap. <i>Physical Review A</i> , <b>2019</b> , 99,	2.6	11
42	Contributions of point defects, chemical disorder, and thermal vibrations to electronic properties of Cd1\( \text{Z}\) TnxTe alloys. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	11
41	Simultaneous control of ionic and electronic conductivity in materials: thallium bromide case study. <i>Physical Review Letters</i> , <b>2012</b> , 108, 246604	7.4	11
40	Theory-guided growth of aluminum antimonide single crystals with optimal properties for radiation detection. <i>Applied Physics Letters</i> , <b>2010</b> , 97, 142104	3.4	9
39	Effects of antimony and ion damage on carrier localization in molecular-beam-epitaxy-grown GalnNAs. <i>Journal of Vacuum Science &amp; Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena</i> , <b>2005</b> , 23, 1320		9
38	Towards probing pentagons on carbon nanotube tips. Surface Science, 1999, 421, L150-L155	1.8	9
37	Magnetic stability of oxygen defects on the SiO2 surface. <i>AIP Advances</i> , <b>2017</b> , 7, 025110	1.5	8
36	Assessing the role of hydrogen in Fermi-level pinning in chalcopyrite and kesterite solar absorbers from first-principles calculations. <i>Journal of Applied Physics</i> , <b>2018</b> , 123, 161408	2.5	8
35	First principles calculation of point defects and mobility degradation in bulk AlSb for radiation detection application <b>2007</b> , 6706, 167		8

## (2021-2019)

34	The role of oxygen doping on elemental intermixing at the PVD-CdS/Cu (InGa)Se2 heterojunction. <i>Progress in Photovoltaics: Research and Applications</i> , <b>2019</b> , 27, 255-263	6.8	7	
33	Radiation Effects on InGaN Quantum Wells and GaN Simultaneously Probed by Ion Beam-Induced Luminescence. <i>IEEE Transactions on Nuclear Science</i> , <b>2008</b> , 55, 3633-3637	1.7	6	
32	Limits on the Existence of sub-MeV Sterile Neutrinos from the Decay of ^{7}Be in Superconducting Quantum Sensors. <i>Physical Review Letters</i> , <b>2021</b> , 126, 021803	7.4	6	
31	Hole traps in sodium silicate: First-principles calculations of the mobility edge. <i>Journal of Non-Crystalline Solids</i> , <b>2015</b> , 430, 9-15	3.9	5	
30	Intermixing and Formation of Cu-Rich Secondary Phases at Sputtered CdS/CuInGaSe2 Heterojunctions. <i>IEEE Journal of Photovoltaics</i> , <b>2016</b> , 6, 1308-1315	3.7	5	
29	Stability of CdZnOS Quaternary Alloys Assessed with First-Principles Calculations. <i>ACS Applied Materials &amp; Discourt &amp; Discourt Materials &amp; Discourt &amp; D</i>	9.5	4	
28	Electronic structure and surface properties of MgB2(0001) upon oxygen adsorption. <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	4	
27	Effect of chlorination on the TlBr band edges for improved room temperature radiation detectors. <i>Physica Status Solidi (B): Basic Research</i> , <b>2015</b> , 252, 1266-1271	1.3	4	
26	Exploring Cd-Zn-O-S alloys for improved buffer layers in thin-film photovoltaics. <i>Physical Review Materials</i> , <b>2017</b> , 1,	3.2	4	
25	A density-functional theory study of the Al/AlOx/Al tunnel junction. <i>Journal of Applied Physics</i> , <b>2020</b> , 128, 155102	2.5	4	
24	Intercalation of Lithium into Graphite: Insights from First-Principles Simulations. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 21985-21992	3.8	4	
23	Materials science for quantum information science and technology. MRS Bulletin, 2020, 45, 485-497	3.2	3	
22	Quantifying Large Lattice Relaxations in Photovoltaic Devices. Physical Review Applied, 2020, 13,	4.3	3	
21	van der Waals-corrected density functional study of electric field noise heating in ion traps caused by electrode surface adsorbates. <i>New Journal of Physics</i> , <b>2019</b> , 21, 053043	2.9	3	
20	Comment on "New Ground-State Crystal Structure of Elemental Boron". <i>Physical Review Letters</i> , <b>2017</b> , 118, 159601	7.4	3	
19	MBE Growth and Characterization of Long Wavelength Dilute Nitride IIII Alloys <b>2005</b> , 1-92		3	
18	The role of water vapor during the synthesis of hydrogen doped In 2 O 3. <i>Applied Physics Letters</i> , <b>2020</b> , 117, 062103	3.4	3	
17	Probing Charge Dynamics in Diamond with an Individual Color Center. <i>Nano Letters</i> , <b>2021</b> , 21, 6960-6966	511.5	3	

16	Amorphous Phase Change Materials: Structure, Stability and Relation with Their Crystalline Phase. <i>Springer Series in Materials Science</i> , <b>2015</b> , 485-509	0.9	2
15	First principles study of the structural, electronic, and optical properties of Sn2+-doped ZnO <b>B</b> 2O5 glasses. <i>Journal of Non-Crystalline Solids</i> , <b>2018</b> , 492, 108-114	3.9	2
14	Cu rich domains and secondary phases in PVD-CdS / PVD-CuIn1\(\mathbb{\mathbb{N}}\)GaxSe2 heterojunctions <b>2015</b> ,		2
13	Understanding Lithium Solvation and Diffusion through Topological Analysis of First-Principles Molecular Dynamics <b>2016</b> ,		2
12	Water ingress mapping in photovoltaic module packaging materials 2018,		2
11	2018,		2
10	HRTEM of Initial Oxidation of Carbon Nanotube Tips. <i>Microscopy and Microanalysis</i> , <b>1997</b> , 3, 421-422	0.5	1
9	Long-wavelength Dilute Nitride-Antimonide Lasers <b>2005</b> , 507-578		1
8	Role of ripples in altering the electronic and chemical properties of graphene <i>Journal of Chemical Physics</i> , <b>2022</b> , 156, 054708	3.9	1
7	Analysis of defects in In2O3:H synthesized in presence of water vapor and hydrogen gas mixture. Journal of Applied Physics, <b>2021</b> , 129, 045102	2.5	1
6	Thermodynamic Modeling of the Al-Ce-Cu-Mg-Si System and Its Application to Aluminum-Cerium Alloy Design. <i>Journal of Phase Equilibria and Diffusion</i> , <b>2020</b> , 41, 764-783	1	0
5	Advances and opportunities in materials science for scalable quantum computing. <i>MRS Bulletin</i> , <b>2021</b> , 46, 589-595	3.2	O
4	Delving into dynamic effects. <i>Nature Chemistry</i> , <b>2020</b> , 12, 225-226	17.6	
3	Photoluminescence and electroabsorption in GaNAstaAsSb heterojunctions. <i>Electronics Letters</i> , <b>2006</b> , 42, 52	1.1	
2	Study Of Single-Wall Carbon Nanotube-Supported Platinum Catalyst For Selective Hydrogenation Of The Carbonyl Function On An (#Unsaturated Aldehyde. <i>Microscopy and Microanalysis</i> , <b>1999</b> , 5, 142-1	43 <sup>0.5</sup>	
1	Behavior of Na and RbF-Treated CdS/Cu(In,Ga)Se2 Solar Cells with Stress Testing under Heat, Light, and Junction Bias. <i>Physica Status Solidi - Rapid Research Letters</i> , <b>2021</b> , 15, 2000530	2.5	