

Giancarlo Trimarchi

List of Publications by Year in descending order

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1405

citing authors

#	ARTICLE	IF	CITATIONS
1	Stereochemical Effects in Supramolecular Self-Assembly at Surfaces: 1-D versus 2-D Enantiomeric Ordering for PVBA and PEBA on Ag(111). <i>Journal of the American Chemical Society</i> , 2002, 124, 7991-8000.	13.7	210
2	Global space-group optimization problem: Finding the stablest crystal structure without constraints. <i>Physical Review B</i> , 2007, 75, .	3.2	148
3	Construction and solution of a Wannier-functions based Hamiltonian in the pseudopotential plane-wave framework for strongly correlated materials. <i>European Physical Journal B</i> , 2008, 65, 91-98.	1.5	96
4	Direct thermal neutron detection by the 2D semiconductor 6LiInP2Se6. <i>Nature</i> , 2020, 577, 346-349.	27.8	59
5	Predicting stable stoichiometries of compounds via evolutionary global space-group optimization. <i>Physical Review B</i> , 2009, 80, .	3.2	54
6	Mesoscopic chiral reshaping of the Ag(110) surface induced by the organic molecule PVBA. <i>Journal of Chemical Physics</i> , 2004, 120, 11367-11370.	3.0	40
7	LDA+DMFT implemented with the pseudopotential plane-wave approach. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 135227 Using design principles to systematically plan the synthesis of hole-conducting transparent oxides: $\text{Cu} \langle \text{mml:math} \text{ xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow}$ $\rangle \langle \text{mml:mn} \rangle 3 \langle / \text{mml:mn} \rangle \langle / \text{mml:msub} \rangle \langle / \text{mml:math} \rangle \text{VO} \langle \text{mml:math}$ $\text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \text{ display="inline"} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow}$ $\rangle \langle \text{mml:mn} \rangle 4 \langle / \text{mml:mn} \rangle \langle / \text{mml:msub} \rangle \langle / \text{mml:math} \rangle \text{and Ag} \langle \text{mml:math}$ $\text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle$	1.8	40
8	Possible pitfalls in theoretical determination of ground-state crystal structures: The case of platinum nitride. <i>Physical Review B</i> , 2009, 79, .	3.2	38
9	Charge Density Wave in the New Polymorphs of $\langle i \rangle \text{RE} \langle /i \rangle \langle \text{sub} \rangle 2 \langle / \text{sub} \rangle \text{Ru} \langle \text{sub} \rangle 3 \langle / \text{sub} \rangle \text{Ge} \langle \text{sub} \rangle 5 \langle / \text{sub} \rangle$ ($\langle i \rangle \text{RE} \langle /i \rangle = \text{Pr, Sm, Dy}$). <i>Journal of the American Chemical Society</i> , 2017, 139, 4130-4143.	13.7	33
10	$\text{CaFe} \langle \text{sub} \rangle 4 \langle / \text{sub} \rangle \text{As} \langle \text{sub} \rangle 3 \langle / \text{sub} \rangle$: A Metallic Iron Arsenide with Anisotropic Magnetic and Charge-Transport Properties. <i>Journal of the American Chemical Society</i> , 2009, 131, 5405-5407.	13.7	32
11	Structural, Optical, and Transport Properties of $\hat{\imath}^{\pm}$ - and $\hat{\imath}^2$ -Ag $\langle \text{sub} \rangle 3 \langle / \text{sub} \rangle \text{VO} \langle \text{sub} \rangle 4 \langle / \text{sub} \rangle$. <i>Chemistry of Materials</i> , 2012, 24, 3346-3354.	6.7	29
12	Strain-Minimizing Tetrahedral Networks of Semiconductor Alloys. <i>Physical Review Letters</i> , 2007, 99, 145501.	7.8	26
13	Finding the lowest-energy crystal structure starting from randomly selected lattice vectors and atomic positions: first-principles evolutionary study of the Au-Pd, Cd-Pt, Al-Sc, Cu-Pd, Pd-Ti, and Ir-N binary systems. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 295212.	1.8	26
14	Structurally unstable $\langle \text{mml:math} \text{ xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:msup} \rangle \langle \text{mml:mi} \rangle \text{A} \langle / \text{mml:mi} \rangle \langle \text{mml:mi} \rangle \text{III} \langle / \text{mml:mi} \rangle \langle / \text{mml:msup} \rangle \langle \text{mml:math}$ $\text{mathvariant="normal"} \rangle \text{BiO} \langle / \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 3 \langle / \text{mml:mn} \rangle \langle / \text{mml:msub} \rangle \langle / \text{mml:math} \rangle$ perovskites are predicted to be topological insulators but their stable structural forms are trivial band insulators. <i>Physical Review B</i> , 2014, 90,	3.2	21
15	Structure prediction and targeted synthesis: A new NanN2 diazenide crystalline structure. <i>Journal of Chemical Physics</i> , 2010, 133, 194504.	3.0	17
16	Substrate-induced supramolecular ordering of functional molecules: theoretical modelling and STM investigation of the PEBA/Ag(111) system. <i>Acta Materialia</i> , 2004, 52, 1589-1595.	7.9	15
17	Prediction and Synthesis of Strain Tolerant RbCuTe Crystals Based on Rotation of One-Dimensional Nano Ribbons within a Three-Dimensional Inorganic Network. <i>Journal of the American Chemical Society</i> , 2015, 137, 11383-11390.	13.7	12

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19	Emergence of a few distinct structures from a single formal structure type during high-throughput screening for stable compounds: The case of RbCuS and RbCuSe. <i>Physical Review B</i> , 2015, 92, .		3.2	10
20	Magnetization of ternary alloys based on Fe0.65Ni0.35 invar with 3 <i>i>d</i></i>	transition metal additions: An <i>< i>ab initio</i></i> study. <i>Journal of Applied Physics</i> , 2015, 117, .	2.5	7
21	Câ€“Fe chains due to segregated carbon impurities on Fe(100). <i>Surface Science</i> , 2006, 600, 3884-3887.		1.9	6
22	KAg11(VO4)4 as a candidate <i>< i>p</i></i> -type transparent conducting oxide. <i>Journal of Chemical Physics</i> , 2013, 138, 194703.		3.0	6
23	Selective Crystal Growth and Structural, Optical, and Electronic Studies of Mn3Ta2O8. <i>Inorganic Chemistry</i> , 2015, 54, 6513-6519.		4.0	6
24	One-dimensional surface states induced by segregated impurities at transition-metal surfaces. <i>Physica Status Solidi (B): Basic Research</i> , 2006, 243, 2105-2110.		1.5	5
25	Long-range order instead of phase separation in large lattice-mismatch isovalent A \tilde{X} B systems. <i>Physical Review B</i> , 2009, 80, .		3.2	5
26	Incomplete Peierls-like chain dimerization as a mechanism for intrinsic conductivity and optical transparency: A La-Cu-O-S phase with mixed-anion layers as a case study. <i>Physical Review B</i> , 2015, 92, .		3.2	4
27	Prediction of ordering and spontaneous rotation of epitaxial habits in substrate-coherent InGaN and GaAsSb. <i>Applied Physics Letters</i> , 2009, 95, 081901.		3.3	3