

SÃ©bastien Le Roux

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/3311413/publications.pdf>

Version: 2024-02-01

21
papers

882
citations

933264

10
h-index

713332

21
g-index

21
all docs

21
docs citations

21
times ranked

975
citing authors

#	ARTICLE	IF	CITATIONS
1	Chalcogenide glasses for innovation in applied science: fundamental issues and new insights. Journal Physics D: Applied Physics, 2020, 53, 033002.	1.3	4
2	Chalcogenide glasses as a playground for the application of first-principles molecular dynamics to disordered materials. Solid State Sciences, 2019, 95, 105925.	1.5	4
3	Sensitivity to Dispersion Forces in First-Principles Modeling of Disordered Chalcogenides. Frontiers in Materials, 2018, 5, .	1.2	7
4	On the occurrence of size effects in the calculation of thermal conductivity by first-principles molecular dynamics: The case of glassy GeTe ₄ . Journal of Non-Crystalline Solids, 2018, 498, 190-193.	1.5	13
5	The role of dispersion forces on the atomic structure of glassy chalcogenides: The case of GeSe ₄ and GeS ₄ . Journal of Non-Crystalline Solids, 2018, 499, 167-172.	1.5	8
6	Structure of amorphous GeSe ₉ by neutron diffraction and first-principles molecular dynamics: Impact of trajectory sampling and size effects. Journal of Chemical Physics, 2016, 145, 084502.	1.2	6
7	Exohedral C ₆₀ and M ₂ C ₆₀ (M = Pt, Pd) systems as tunable-gap building blocks for nanoarchitecture and nanocatalysis. Journal of Chemical Physics, 2015, 143, 114308.	1.2	6
8	Origin of structural analogies and differences between the atomic structures of GeSe ₄ and GeS ₄ glasses: A first principles study. Journal of Chemical Physics, 2015, 143, 034504.	1.2	35
9	Density-driven defect-mediated network collapse of GeSe ₂ glass. Physical Review B, 2014, 90, .	1.1	30
10	Metal-organic molecule-metal nano-junctions: a close contact between first-principles simulations and experiments. Journal of Physics Condensed Matter, 2014, 26, 104206.	0.7	7
11	The structure of liquid GeSe revisited: A first principles molecular dynamics study. Journal of Chemical Physics, 2013, 138, 174505.	1.2	21
12	Structural properties of glassy GeSe ₃ from first-principles molecular dynamics. Physical Review B, 2012, 86, .	1.1	33
13	Network connectivity and extended Se chains in the atomic structure of glassy GeSe ₄ . Chemical Physics Letters, 2012, 547, 30-34.	1.2	16
14	Investigation of size effects on the structure of liquid GeSe ₂ calculated via first-principles molecular dynamics. Journal of Chemical Physics, 2012, 136, 224504.	1.2	20
15	Three-dimensional structure of multicomponent (Na ₂ O) _{0.35} [(P ₂ O ₅) ₁ x (B ₂ O ₃) ₃] _{0.65} glasses by high-energy x-ray diffraction and constrained reverse Monte Carlo simulations. Journal of Physics	0.7	8
16	Structural properties of liquid GeSe ₂ from first-principles molecular dynamics. Physical Review B, 2011, 84, .	1.1	22
17	ISAACS interactive structure analysis of amorphous and crystalline systems. Journal of Applied Crystallography, 2010, 43, 181-185.	1.9	242
18	Ring statistics analysis of topological networks: New approach and application to amorphous GeS ₂ and SiO ₂ systems. Computational Materials Science, 2010, 49, 70-83.	1.4	387

#	ARTICLE	IF	CITATIONS
19	On the influence of the initial liquid configuration on the structure of a glass obtained using ab-initio molecular dynamics simulations. Journal of Non-Crystalline Solids, 2009, 355, 1807-1810.	1.5	1
20	<i>Ab initio</i> molecular dynamics study of GeS ₂ : from the crystal to the glass. Journal of Physics Condensed Matter, 2007, 19, 455207.	0.7	3
21	Influence of the cooling rate on the glass transition temperature and the structural properties of glassy GeS ₂ : an ab initio molecular dynamics study. Journal of Physics Condensed Matter, 2007, 19, 196102.	0.7	9