SÃ©bastien Le Roux

List of Publications by Year
in descending order

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

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21	882	933264	713332
papers	citations	10 h-index	21 g-index

21	21	21	975
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ring statistics analysis of topological networks: New approach and application to amorphous GeS2 and SiO2 systems. Computational Materials Science, 2010, 49, 70-83.	1.4	387
2	ISAACSâ€“ interactive structure analysis of amorphous and crystalline systems. Journal of Applied Crystallography, 2010, 43, 181-185.	1.9	242
3	Origin of structural analogies and differences between the atomic structures of GeSe4 and GeS4 glasses: A first principles study. Journal of Chemical Physics, 2015, 143, 034504.	1.2	35
4	Structural properties of glassy Ge<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Se<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>from first-principles molecular dynamics. Physical Review B, 2012, 86, .	1.1	33
5	Density-driven defect-mediated network collapse of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">GeSe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>glass. Physical Review B, 2014, 90, .	1.1	30
6	Structural properties of liquid Ge<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Se<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>: A first-principles study. Physical Review B, 2011, 84, .	1.1	22
7	The structure of liquid GeSe revisited: A first principles molecular dynamics study. Journal of Chemical Physics, 2013, 138, 174505.	1.2	21
8	Investigation of size effects on the structure of liquid GeSe2 calculated via first-principles molecular dynamics. Journal of Chemical Physics, 2012, 136, 224504.	1.2	20
9	Network connectivity and extended Se chains in the atomic structure of glassy GeSe4. Chemical Physics Letters, 2012, 547, 30-34.	1.2	16
10	On the occurrence of size effects in the calculation of thermal conductivity by first-principles molecular dynamics: The case of glassy GeTe4. Journal of Non-Crystalline Solids, 2018, 498, 190-193.	1.5	13
11	Influence of the cooling rate on the glass transition temperature and the structural properties of glassy GeS2: anab initiomolecular dynamics study. Journal of Physics Condensed Matter, 2007, 19, 196102.	0.7	9
12	Three-dimensional structure of multicomponent (Na₂O)_{0.35}[(P₂O₅)_{1 â^’x}(B₂O₃)_x]_{0.65}glasses by high-energy x-ray diffraction and constrained reverse Monte Carlo simulations. Journal of Physics Condensed Matter, 2011, 23, 035403.	0.7	8
13	The role of dispersion forces on the atomic structure of glassy chalcogenides: The case of GeSe4 and GeS4. Journal of Non-Crystalline Solids, 2018, 499, 167-172.	1.5	8
14	Metalâ€“organic moleculeâ€“metal nano-junctions: a close contact between first-principles simulations and experiments. Journal of Physics Condensed Matter, 2014, 26, 104206.	0.7	7
15	Sensitivity to Dispersion Forces in First-Principles Modeling of Disordered Chalcogenides. Frontiers in Materials, 2018, 5, .	1.2	7
16	Exohedral Mâ€“C60 and M2â€“C60 (M = Pt, Pd) systems as tunable-gap building blocks for nanoarchitecture and nanocatalysis. Journal of Chemical Physics, 2015, 143, 114308.	1.2	6
17	Structure of amorphous GeSe9 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
18	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

#	Article	IF	Citations
19	Chalcogenide glasses for innovation in applied science: fundamental issues and new insights. Journal Physics D: Applied Physics, 2020, 53, 033002.	1.3	4
20	Ab initiomolecular dynamics study of GeS₂: from the crystal to the glass. Journal of Physics Condensed Matter, 2007, 19, 455207.	0.7	3
21	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