Natalie Holzwarth

List of Publications by Year
in descending order

22 papers	2,366 citations	840776 11 h-index	752698 20 g-index
22 all docs	22 docs citations	22 times ranked	4037 citing authors

#	Article	IF	Citations
1	First-principles simulations of Li boracites <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Li</mml:mi><mml:mn>4</mml:mn></mm… mathvariant="normal">B</mml:mi><mml:mn>7</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>12</mml:mn></mml:msub><mml:mi>Cl</mml:mi></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Li</mml:mi><mml:mn>5</mml:mn></mml:…	2.4	3
2	Cubic spline solver for generalized density functional treatments of atoms and generation of atomic datasets for use with exchange-correlation functionals including meta-GGA. Physical Review B, 2022, 105, .	3.2	9
3	First-principles simulations to understand the structural and electrolyte properties of idealized <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Li</mml:mi><mml:mrow><mml:mn>7.5</… mathvariant="normal">B</mml:mi><mml:mn>10</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>18</mml:mn></mml:msub><mml:msub><mml:mi>X</mml:mi><mml:mrow><mml:mn>1… <mi… Physical Review Materials, 2022, 6, .	2.4	3
4	Computational study of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Li</mml:mi><mml:mn>3</mml:mn></mml:… and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Li</mml:mi><mml:mn>3</mml:mn></mml:… Stability analysis of pure phases and of model interfaces with Li. Physical Review Materials, 2021, 5, .	2.4	4
5	Computational study of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Li</mml:mi><mml:mn>3</mml:mn></mm… and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Li</mml:mi><mml:mn>3</mml:mn></mm… I: Electrolyte properties of pure and doped crystals. Physical Review Materials, 2021, 5, .	2.4	3
6	Computational Investigation of Known and Predicted Li Boracites Li4B7O12Cl and Li4B7S12Cl as Solid Electrolytes Having Possible Applications for Developing All Solid-state Li Ion Batteries. ECS Meeting Abstracts, 2021, MA2021-02, 255-255.	0.0	0
7	First Principles Simulations to Understand the Structural and Electrolyte Properties of Idealized Li7.5B10S18X1.5 (X = Cl, Br, I) Li Superionic Conductors Recently Identified in the Experimental Literature. ECS Meeting Abstracts, 2021, MA2021-02, 256-256.	0.0	0
8	The Abinitproject: Impact, environment and recent developments. Computer Physics Communications, 2020, 248, 107042.	7.5	369
9	Continuity of phonon dispersion curves in layered ionic materials. Journal of Physics Condensed Matter, 2020, 32, 055402.	1.8	2
10	Computational and experimental (re)investigation of the structural and electrolyte properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Li</mml:mi><mml:mn>4</mml:mn></mml:… mathvariant="normal">P</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>6</mml:mn></mml:msub></mml:mrow><mml:mo>,</mml:mo><mml:mo>Â</mml:mo><… Physical Review Materials, 2020, 4, .	2.4	4
11	Unraveling the electrolyte properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Na</mml:mi><mml:mn>3</mml:mn></m… through computation and experiment. Physical Review Materials, 2017, 1, .	2.3	21
12	Fundamental aspects of the structural and electrolyte properties of Li2OHCl from simulations and experiment. Physical Review Materials, 2017, 1, .	2.4	36
13	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
14	Modeling interfaces between solids: Application to Li battery materials. Physical Review B, 2015, 92, .	3.2	68
15	Crystalline Inorganic Solid Electrolytes: Computer Simulations and Comparisons with Experiment. Materials and Energy, 2015, , 191-232.	0.1	1
16	Cu2ZnSnS<i>x</i>O4â^ˆ’<i>x</i> and Cu2ZnSnS<i>x</i>Se4â^ˆ’<i>x</i>: First principles simulations of optimal alloy configurations and their energies. Journal of Applied Physics, 2014, 115, .	2.5	22
17	Generation of Projector Augmented-Wave atomic data: A 71 element validated table in the XML format. Computer Physics Communications, 2014, 185, 1246-1254.	7.5	202
18	Structures, Li<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mrow /><mml:mo>+</mml:mo></mml:msup></mml:math>mobilities, and interfacial properties of solid electrolytes Li<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>PS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:	3.2	138

#	Article	IF	Citations
19	Computer Modeling of Crystalline Electrolytes: Lithium Thiophosphates and Phosphates. Journal of the Electrochemical Society, 2012, 159, A538-A547.	2.9	41
20	First Principles Simulations of Li Ion Migration in Materials Related to LiPON Electrolytes. ECS Transactions, 2010, 25, 27-36.	0.5	4
21	Mechanisms of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi mathvariant="normal">Li</mml:mi><mml:mo>+</mml:mo></mml:msup></mml:math>diffusion in crystalline<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î³</mml:mi></mml:math>- and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow></mml:mrow><mml:mi></mml:mi>	3.2	93
22	Comparison of the projector augmented-wave, pseudopotential, and linearized augmented-plane-wave formalisms for density-functional calculations of solids. Physical Review B, 1997, 55, 2005-2017.	3.2	230