

Jan W Andzelm

List of Publications by Year in descending order

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33
papers

1,304
citations

394421

19
h-index

377865

34
g-index

34
all docs

34
docs citations

34
times ranked

1677
citing authors

#	ARTICLE	IF	CITATIONS
1	Geometry optimization of solids using delocalized internal coordinates. <i>Chemical Physics Letters</i> , 2001, 335, 321-326.	2.6	167
2	AIREBO-M: A reactive model for hydrocarbons at extreme pressures. <i>Journal of Chemical Physics</i> , 2015, 142, 024903.	3.0	159
3	Mechanical and Structural Characterization of Semicrystalline Polyethylene under Tensile Deformation by Molecular Dynamics Simulations. <i>Macromolecules</i> , 2015, 48, 4228-4239.	4.8	111
4	High strain rate mechanical properties of a cross-linked epoxy across the glass transition. <i>Polymer</i> , 2013, 54, 7048-7057.	3.8	94
5	Interface binding and mechanical properties of MXene-epoxy nanocomposites. <i>Composites Science and Technology</i> , 2020, 192, 108124.	7.8	64
6	Molecular Dynamics Simulation of the Effects of Layer Thickness and Chain Tilt on Tensile Deformation Mechanisms of Semicrystalline Polyethylene. <i>Macromolecules</i> , 2017, 50, 1700-1712.	4.8	57
7	Ordering and Crystallization of Entangled Polyethylene Melts under Uniaxial Tension: A Molecular Dynamics Study. <i>Macromolecules</i> , 2018, 51, 9635-9648.	4.8	49
8	Shock Hugoniot calculations of polymers using quantum mechanics and molecular dynamics. <i>Journal of Chemical Physics</i> , 2012, 137, 204901.	3.0	46
9	Fast protocol for equilibration of entangled and branched polymer chains. <i>Chemical Physics Letters</i> , 2012, 523, 139-143.	2.6	45
10	First Principles Modeling of Water Dissociation on Mg(0001) and Development of a Mg Surface Pourbaix Diagram. <i>Corrosion</i> , 2015, 71, 209-223.	1.1	45
11	Modeling reaction pathways for hydrogen evolution and water dissociation on magnesium. <i>Electrochimica Acta</i> , 2016, 210, 261-270.	5.2	44
12	Modeling viscoelastic properties of triblock copolymers: A DPD simulation study. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2010, 48, 15-25.	2.1	40
13	Exploring the ability of a multiscale coarse-grained potential to describe the stress-strain response of glassy polystyrene. <i>Physical Review E</i> , 2013, 87, 042606.	2.1	40
14	Effect of polymer solvent on the mechanical properties of entangled polymer gels: Coarse-grained molecular simulation. <i>Polymer</i> , 2013, 54, 2555-2564.	3.8	37
15	Computational study of thermal and mechanical properties of nylons and bio-based furan polyamides. <i>Polymer</i> , 2014, 55, 166-174.	3.8	37
16	A molecular simulation study of the glass transition of cross-linked poly(dicyclopentadiene) networks. <i>Chemical Physics Letters</i> , 2015, 637, 103-109.	2.6	34
17	First Principles Modeling of Cathodic Reaction Thermodynamics in Dilute Magnesium Alloys. <i>Corrosion</i> , 2017, 73, 506-517.	1.1	27
18	High strength films from oriented, hydrogen-bonded α -graphamid \cdot 2D polymer molecular ensembles. <i>Scientific Reports</i> , 2018, 8, 3708.	3.3	24

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19	Phase behavior of SEBS triblock copolymer gels. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2011, 49, 1479-1491.	2.1	20
20	Molecular origins of anisotropic shock propagation in crystalline and amorphous polyethylene. <i>Physical Review Materials</i> , 2018, 2, .	2.4	18
21	Role of entanglements and bond scission in high strain-rate deformation of polymer gels. <i>Polymer</i> , 2014, 55, 2543-2551.	3.8	17
22	Coarse-grained modeling of model poly(urethane urea)s: Microstructure and interface aspects. <i>Polymer</i> , 2012, 53, 4512-4524.	3.8	15
23	Structural and mechanical properties of advanced polymer gels with rigid side-chains using coarse-grained molecular dynamics. <i>Polymer</i> , 2014, 55, 5266-5275.	3.8	15
24	Shock-wave propagation and reflection in semicrystalline polyethylene: A molecular-level investigation. <i>Physical Review Materials</i> , 2017, 1, .	2.4	15
25	Vibrational Analysis of Semicrystalline Polyethylene Using Molecular Dynamics Simulation. <i>Macromolecules</i> , 2017, 50, 6690-6701.	4.8	12
26	Use of 3-aminopropyltriethoxysilane deposited from aqueous solution for surface modification of III-V materials. <i>Applied Surface Science</i> , 2014, 320, 414-428.	6.1	11
27	First principles investigation of water adsorption and charge transfer on III-V(110) semiconductor surfaces. <i>Surface Science</i> , 2014, 622, 71-82.	1.9	10
28	Computational Study of Structural and Energetic Properties of Ammonium Perchlorate at Interfaces. <i>Journal of Physical Chemistry C</i> , 2021, 125, 12297-12304.	3.1	9
29	Calculations of free energy of surface interactions in crystalline polyethylene. <i>Journal of Chemical Physics</i> , 2018, 149, 014701.	3.0	6
30	Effects of Finite Lengths of Chains on the Structural and Mechanical Properties of Polyethylene Fibers. <i>Macromolecules</i> , 2020, 53, 18-28.	4.8	6
31	Chemical and physical passivation of type II strained-layer superlattice devices by means of thiolated self-assembled monolayers and polymer encapsulates. <i>Infrared Physics and Technology</i> , 2015, 70, 48-52.	2.9	5
32	Bonding of cysteamine on InAs surfaces. <i>Applied Surface Science</i> , 2018, 462, 489-501.	6.1	5
33	Highly Thermostable Dynamic Structures of Polyaramid Two-Dimensional Polymers. <i>Macromolecules</i> , 2021, 54, 1291-1303.	4.8	3