# Jan W Andzelm

List of Publications by Year
in descending order

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| 33 | 1,304 | 394421 | 377865 |
|---|---|---|---|
| papers | citations | 19 h-index | 34 g-index |

| 34 | 34 | 34 | 1677 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Computational Study of Structural and Energetic Properties of Ammonium Perchlorate at Interfaces. Journal of Physical Chemistry C, 2021, 125, 12297-12304. | 3.1 | 9 |
| 2 | Highly Thermostable Dynamic Structures of Polyaramid Two-Dimensional Polymers. Macromolecules, 2021, 54, 1291-1303. | 4.8 | 3 |
| 3 | Effects of Finite Lengths of Chains on the Structural and Mechanical Properties of Polyethylene Fibers. Macromolecules, 2020, 53, 18-28. | 4.8 | 6 |
| 4 | Interface binding and mechanical properties of MXene-epoxy nanocomposites. Composites Science and Technology, 2020, 192, 108124. | 7.8 | 64 |
| 5 | High strength films from oriented, hydrogen-bonded â€œgraphamidâ€•2D polymer molecular ensembles. Scientific Reports, 2018, 8, 3708. | 3.3 | 24 |
| 6 | Ordering and Crystallization of Entangled Polyethylene Melts under Uniaxial Tension: A Molecular Dynamics Study. Macromolecules, 2018, 51, 9635-9648. | 4.8 | 49 |
| 7 | Bonding of cysteamine on InAs surfaces. Applied Surface Science, 2018, 462, 489-501. | 6.1 | 5 |
| 8 | Calculations of free energy of surface interactions in crystalline polyethylene. Journal of Chemical Physics, 2018, 149, 014701. | 3.0 | 6 |
| 9 | Molecular origins of anisotropic shock propagation in crystalline and amorphous polyethylene. Physical Review Materials, 2018, 2, . | 2.4 | 18 |
| 10 | Molecular Dynamics Simulation of the Effects of Layer Thickness and Chain Tilt on Tensile Deformation Mechanisms of Semicrystalline Polyethylene. Macromolecules, 2017, 50, 1700-1712. | 4.8 | 57 |
| 11 | First Principles Modeling of Cathodic Reaction Thermodynamics in Dilute Magnesium Alloys. Corrosion, 2017, 73, 506-517. | 1.1 | 27 |
| 12 | Vibrational Analysis of Semicrystalline Polyethylene Using Molecular Dynamics Simulation. Macromolecules, 2017, 50, 6690-6701. | 4.8 | 12 |
| 13 | Shock-wave propagation and reflection in semicrystalline polyethylene: A molecular-level investigation. Physical Review Materials, 2017, 1, . | 2.4 | 15 |
| 14 | Modeling reaction pathways for hydrogen evolution and water dissociation on magnesium. Electrochimica Acta, 2016, 210, 261-270. | 5.2 | 44 |
| 15 | AIREBO-M: A reactive model for hydrocarbons at extreme pressures. Journal of Chemical Physics, 2015, 142, 024903. | 3.0 | 159 |
| 16 | First Principles Modeling of Water Dissociation on Mg(0001) and Development of a Mg Surface Pourbaix Diagram. Corrosion, 2015, 71, 209-223. | 1.1 | 45 |
| 17 | Mechanical and Structural Characterization of Semicrystalline Polyethylene under Tensile Deformation by Molecular Dynamics Simulations. Macromolecules, 2015, 48, 4228-4239. | 4.8 | 111 |
| 18 | A molecular simulation study of the glass transition of cross-linked poly(dicyclopentadiene) networks. Chemical Physics Letters, 2015, 637, 103-109. | 2.6 | 34 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Chemical and physical passivation of type II strained-layer superlattice devices by means of thiolated self-assembled monolayers and polymer encapsulates. Infrared Physics and Technology, 2015, 70, 48-52. | 2.9 | 5 |
| 20 | Computational study of thermal and mechanical properties of nylons and bio-based furan polyamides. Polymer, 2014, 55, 166-174. | 3.8 | 37 |
| 21 | First principles investigation of water adsorption and charge transfer on IIIâ€“V(110) semiconductor surfaces. Surface Science, 2014, 622, 71-82. | 1.9 | 10 |
| 22 | Structural and mechanical properties of advanced polymer gels with rigid side-chains using coarse-grained molecular dynamics. Polymer, 2014, 55, 5266-5275. | 3.8 | 15 |
| 23 | Use of 3-aminopropyltriethoxysilane deposited from aqueous solution for surface modification of III-V materials. Applied Surface Science, 2014, 320, 414-428. | 6.1 | 11 |
| 24 | Role of entanglements and bond scission in high strain-rate deformation of polymer gels. Polymer, 2014, 55, 2543-2551. | 3.8 | 17 |
| 25 | High strain rate mechanical properties of a cross-linked epoxy across the glass transition. Polymer, 2013, 54, 7048-7057. | 3.8 | 94 |
| 26 | Effect of polymer solvent on the mechanical properties of entangled polymer gels: Coarse-grained molecular simulation. Polymer, 2013, 54, 2555-2564. | 3.8 | 37 |
| 27 | Exploring the ability of a multiscale coarse-grained potential to describe the stress-strain response of glassy polystyrene. Physical Review E, 2013, 87, 042606. | 2.1 | 40 |
| 28 | Coarse-grained modeling of model poly(urethane urea)s: Microstructure and interface aspects. Polymer, 2012, 53, 4512-4524. | 3.8 | 15 |
| 29 | Shock Hugoniot calculations of polymers using quantum mechanics and molecular dynamics. Journal of Chemical Physics, 2012, 137, 204901. | 3.0 | 46 |
| 30 | Fast protocol for equilibration of entangled and branched polymer chains. Chemical Physics Letters, 2012, 523, 139-143. | 2.6 | 45 |
| 31 | Phase behavior of SEBS triblock copolymer gels. Journal of Polymer Science, Part B: Polymer Physics, 2011, 49, 1479-1491. | 2.1 | 20 |
| 32 | Modeling viscoelastic properties of triblock copolymers: A DPD simulation study. Journal of Polymer Science, Part B: Polymer Physics, 2010, 48, 15-25. | 2.1 | 40 |
| 33 | Geometry optimization of solids using delocalized internal coordinates. Chemical Physics Letters, 2001, 335, 321-326. | 2.6 | 167 |