# Raymundo Arroyave

List of Publications by Year
in descending order



| 203 | 6,284 | 61857 | 98622 |
|---|---|---|---|
| papers | citations | 43 h-index | 67 g-index |

| 209 | 209 | 209 | 5059 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Bayesian Calibration of Multiple Coupled Simulation Models for Metal Additive Manufacturing: A Bayesian Network Approach. ASCE-ASME Journal of Risk and Uncertainty in Engineering Systems, Part B: Mechanical Engineering, 2022, 8, . | 0.7 | 5 |
| 2 | Data Science, Machine Learning and Artificial Intelligence Applied to Metals and Alloys Research: Past, Present, and Future. , 2022, , 609-621. | | 2 |
| 3 | On the importance of microstructure information in materials design: PSP vs PP. Acta Materialia, 2022, 223, 117471. | 3.8 | 11 |
| 4 | Microstructure classification in the unsupervised context. Acta Materialia, 2022, 223, 117434. | 3.8 | 10 |
| 5 | Towards stacking fault energy engineering in FCC high entropy alloys. Acta Materialia, 2022, 224, 117472. | 3.8 | 44 |
| 6 | A differential evaporation model to predict chemistry change of additively manufactured metals. Materials and Design, 2022, 213, 110328. | 3.3 | 4 |
| 7 | Machine learning-assisted high-throughput exploration of interface energy space in multi-phase-field model with CALPHAD potential. Materials Theory, 2022, 6, . | 2.2 | 5 |
| 8 | Machine-learning enabled thermodynamic model for the design of new rare-earth compounds. Acta Materialia, 2022, 229, 117759. | 3.8 | 13 |
| 9 | Laser Powder Bed Fusion of Defect-Free NiTi Shape Memory Alloy Parts with Superior Tensile Superelasticity. Acta Materialia, 2022, 229, 117781. | 3.8 | 79 |
| 10 | Efficient machine-learning model for fast assessment of elastic properties of high-entropy alloys. Acta Materialia, 2022, 232, 117924. | 3.8 | 39 |
| 11 | Hybrid microstructure-defect printability map in laser powder bed fusion additive manufacturing. Computational Materials Science, 2022, 209, 111401. | 1.4 | 5 |
| 12 | Review: additive manufacturing of pure tungsten and tungsten-based alloys. Journal of Materials Science, 2022, 57, 9769-9806. | 1.7 | 8 |
| 13 | Accelerated materials design using batch Bayesian optimization: A case study for solving the inverse problem from materials microstructure to process specification. Computational Materials Science, 2022, 210, 111417. | 1.4 | 10 |
| 14 | Predicting Van der Waals Heterostructures by a Combined Machine Learning and Density Functional Theory Approach. ACS Applied Materials & Interfaces, 2022, 14, 25907-25919. | 4.0 | 8 |
| 15 | Multi-objective materials bayesian optimization with active learning of design constraints: Design of ductile refractory multi-principal-element alloys. Acta Materialia, 2022, 236, 118133. | 3.8 | 22 |
| 16 | Metric-driven search for structurally stable inorganic compounds. Acta Materialia, 2021, 202, 437-447. | 3.8 | 6 |
| 17 | Effect of Pd alloying on structural, electronic and magnetic properties of L10 Feâ€“Ni. Journal of Physics Condensed Matter, 2021, 33, 154003. | 0.7 | 0 |
| 18 | Laser-based additive manufacturing of a binary Ni-5â€‰wt.%Nb alloy. Journal of Manufacturing Processes, 2021, 62, 720-728. | 2.8 | 7 |

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| 19 | Microstructure-Based Modeling of the Effect of Inclusion on the Bendability of Advanced High Strength Dual-Phase Steels. Metals, 2021, 11, 431. | 1.0 | 5 |
| 20 | A Top-Down Characterization of NiTi Single-Crystal Inelastic Properties within Confidence Bounds through Bayesian Inference. Shape Memory and Superelasticity, 2021, 7, 50-64. | 1.1 | 5 |
| 21 | Competing Interactions between Mesoscale Length-Scales, Order-Disorder, and Martensitic Transformation in Ferromagnetic Shape Memory Alloys. Acta Materialia, 2021, 206, 116616. | 3.8 | 16 |
| 22 | Efficiently exploiting process-structure-property relationships in material design by multi-information source fusion. Acta Materialia, 2021, 206, 116619. | 3.8 | 18 |
| 23 | High temperature oxidation behavior of disordered (Ti0.5Zr0.5)2AlC MAX phase via a Machine Learning-Augmented DFT approach. Materials Letters: X, 2021, 10, 100062. | 0.3 | 1 |
| 24 | A printability assessment framework for fabricating low variability nickel-niobium parts using laser powder bed fusion additive manufacturing. Rapid Prototyping Journal, 2021, 27, 1737-1748. | 1.6 | 6 |
| 25 | Controlling martensitic transformation characteristics in defect-free NiTi shape memory alloys fabricated using laser powder bed fusion and a process optimization framework. Acta Materialia, 2021, 215, 117017. | 3.8 | 78 |
| 26 | Martensitic Transformation in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:msub><mml:mrow><mml:mi>Fe</mml:mi></mml:mrow><mml:mrow><mml:mi>x</mml:mi> Physical Review Letters, 2021, 127, 115704. | 2.9 | 12 |
| 27 | An efficient framework for printability assessment in Laser Powder Bed Fusion metal additive manufacturing. Additive Manufacturing, 2021, 46, 102018. | 1.7 | 9 |
| 28 | Effect of composition and phase diagram features on printability and microstructure in laser powder bed fusion: Development and comparison of processing maps across alloy systems. Additive Manufacturing, 2021, 47, 102258. | 1.7 | 3 |
| 29 | A rigorous test and improvement of the Eagar-Tsai model for melt pool characteristics in laser powder bed fusion additive manufacturing. Additive Manufacturing, 2021, 47, 102300. | 1.7 | 2 |
| 30 | Effect of heat treatments on the microstructure and mechanical properties of an ultra-high strength martensitic steel fabricated via laser powder bed fusion additive manufacturing. Additive Manufacturing, 2021, 47, 102255. | 1.7 | 7 |
| 31 | Adaptive active subspace-based efficient multifidelity materials design. Materials and Design, 2021, 209, 110001. | 3.3 | 17 |
| 32 | Incommensurate transition-metal dichalcogenides via mechanochemical reshuffling of binary precursors. Nanoscale Advances, 2021, 3, 4065-4071. | 2.2 | 4 |
| 33 | High-throughput reaction engineering to assess the oxidation stability of MAX phases. Npj Computational Materials, 2021, 7, . | 3.5 | 13 |
| 34 | Computational Design of Compositionally Graded Alloys for Property Monotonicity. Journal of Mechanical Design, Transactions of the ASME, 2021, 143, . | 1.7 | 4 |
| 35 | The BAREFOOT Optimization Framework. Integrating Materials and Manufacturing Innovation, 2021, 10, 644-660. | 1.2 | 4 |
| 36 | Bayesian optimization with adaptive surrogate models for automated experimental design. Npj Computational Materials, 2021, 7, . | 3.5 | 27 |

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| 37 | Nanocalorimetry and ab initio study of ternary elements in CuZr-based shape memory alloy. Acta Materialia, 2020, 182, 29-38. | 3.8 | 9 |
| 38 | Bayesian probabilistic prediction of precipitation behavior in Ni-Ti shape memory alloys. Computational Materials Science, 2020, 172, 109334. | 1.4 | 9 |
| 39 | Mapping mechanisms and growth regimes of magnesium electrodeposition at high current densities. Materials Horizons, 2020, 7, 843-854. | 6.4 | 77 |
| 40 | An ultra-high strength martensitic steel fabricated using selective laser melting additive manufacturing: Densification, microstructure, and mechanical properties. Acta Materialia, 2020, 186, 199-214. | 3.8 | 151 |
| 41 | Design of alumina-forming austenitic stainless steel using genetic algorithms. Materials and Design, 2020, 186, 108198. | 3.3 | 15 |
| 42 | The effect of chemical disorder on defect formation and migration in disordered max phases. Acta Materialia, 2020, 184, 50-58. | 3.8 | 15 |
| 43 | Finite interface dissipation phase field modeling of Niâ€“Nb under additive manufacturing conditions. Acta Materialia, 2020, 185, 320-339. | 3.8 | 83 |
| 44 | On the complexity of solid-state diffusion in highly concentrated alloys and the sluggish diffusion core-effect. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2020, 68, 101713. | 0.7 | 17 |
| 45 | Uncertainty propagation in a multiscale CALPHAD-reinforced elastochemical phase-field model. Acta Materialia, 2020, 183, 452-470. | 3.8 | 23 |
| 46 | Navigating the design space of inorganic materials synthesis using statistical methods and machine learning. Dalton Transactions, 2020, 49, 11480-11488. | 1.6 | 24 |
| 47 | Atomic Hourglass and Thermometer Based on Diffusion of a Mobile Dopant in VO<sub>2</sub>. Journal of the American Chemical Society, 2020, 142, 15513-15526. | 6.6 | 23 |
| 48 | Phase-Field Study of Thermomigration in 3-D IC Micro Interconnects. IEEE Transactions on Components, Packaging and Manufacturing Technology, 2020, 10, 1466-1473. | 1.4 | 6 |
| 49 | Materials Design Through Batch Bayesian Optimization with Multisource Information Fusion. Jom, 2020, 72, 4431-4443. | 0.9 | 15 |
| 50 | Impact of particle arrays on phase separation composition patterns. Journal of Chemical Physics, 2020, 152, 224902. | 1.2 | 7 |
| 51 | Investigation of the discontinuous precipitation of U-Nb alloys via thermodynamic analysis and phase-field modeling. Computational Materials Science, 2020, 175, 109573. | 1.4 | 13 |
| 52 | Uncertainty Quantification and Propagation in Computational Materials Science and Simulation-Assisted Materials Design. Integrating Materials and Manufacturing Innovation, 2020, 9, 103-143. | 1.2 | 35 |
| 53 | Semi-supervised learning approaches to class assignment in ambiguous microstructures. Acta Materialia, 2020, 188, 49-62. | 3.8 | 24 |
| 54 | Statistical modelling of microsegregation in laser powder-bed fusion. Philosophical Magazine Letters, 2020, 100, 271-282. | 0.5 | 4 |

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| 55 | Intellectual Community as a Bridge of Interdisciplinary Graduate Education in Materials Data Science. MRS Advances, 2020, 5, 355-362. | 0.5 | 0 |
| 56 | Accelerated design of Fe-based soft magnetic materials using machine learning and stochastic optimization. Acta Materialia, 2020, 194, 144-155. | 3.8 | 60 |
| 57 | Uncertainty analysis of microsegregation during laser powder bed fusion. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 034002. | 0.8 | 14 |
| 58 | Functionally Graded Materials through robotics-inspired path planning. Materials and Design, 2019, 182, 107975. | 3.3 | 28 |
| 59 | Assessing printability maps in additive manufacturing of metal alloys. Acta Materialia, 2019, 176, 199-210. | 3.8 | 146 |
| 60 | Efficient use of multiple information sources in material design. Acta Materialia, 2019, 180, 260-271. | 3.8 | 21 |
| 61 | Uncertainty Propagation via Probability Measure Optimized Importance Weights with Application to Parametric Materials Models. , 2019, , . | | 4 |
| 62 | Experiment Design Frameworks for Accelerated Discovery of Targeted Materials Across Scales. Frontiers in Materials, 2019, 6, . | 1.2 | 21 |
| 63 | Exploration of the microstructure space in TiAlZrN ultra-hard nanostructured coatings. Acta Materialia, 2019, 174, 459-476. | 3.8 | 16 |
| 64 | Uncertainty quantification and propagation in CALPHAD modeling. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 034003. | 0.8 | 14 |
| 65 | Uncertainty quantification of the parameters and predictions of a phenomenological constitutive model for thermally induced phase transformation in Niâ€“Ti shape memory alloys. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 034001. | 0.8 | 12 |
| 66 | Systems Approaches to Materials Design: Past, Present, and Future. Annual Review of Materials Research, 2019, 49, 103-126. | 4.3 | 49 |
| 67 | Machine Learning-Directed Navigation of Synthetic Design Space: A Statistical Learning Approach to Controlling the Synthesis of Perovskite Halide Nanoplatelets in the Quantum-Confined Regime. Chemistry of Materials, 2019, 31, 3281-3292. | 3.2 | 40 |
| 68 | Design of multifunctional supercapacitor electrodes using an informatics approach. Molecular Systems Design and Engineering, 2019, 4, 654-663. | 1.7 | 17 |
| 69 | On the fast kinetics of B2â€“L21 ordering in Ni-Co-Mn-In metamagnetic shape memory alloys. Journal of Alloys and Compounds, 2019, 781, 479-489. | 2.8 | 10 |
| 70 | Bayesian uncertainty quantification and information fusion in CALPHAD-based thermodynamic modeling. Acta Materialia, 2019, 164, 636-647. | 3.8 | 41 |
| 71 | A proof of concept: Thermodynamics of aluminum â€“ transition metal highly concentrated alloys. Journal of Alloys and Compounds, 2019, 781, 595-605. | 2.8 | 10 |
| 72 | Effects of composition and crystallographic ordering on the ferromagnetic transition in Ni Co Mn In magnetic shape memoryÂalloys. Acta Materialia, 2019, 166, 630-637. | 3.8 | 8 |

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| 73 | Processing of novel pseudomorphic Cuâ€“Mo hierarchies in thin films. Materials Research Letters, 2019, 7, 1-11. | 4.1 | 26 |
| 74 | Numerical and experimental analysis of heat distribution in the laser powder bed fusion of Ti-6Al-4V. IISE Transactions, 2019, 51, 136-152. | 1.6 | 62 |
| 75 | Efficient exploration of the High Entropy Alloy composition-phase space. Acta Materialia, 2018, 152, 41-57. | 3.8 | 62 |
| 76 | Microstructural refinement in an ultra-high strength martensitic steel via equal channel angular pressing. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2018, 725, 57-64. | 2.6 | 29 |
| 77 | Probing the entropy hypothesis in highly concentrated alloys. Acta Materialia, 2018, 148, 263-279. | 3.8 | 39 |
| 78 | Probing Structural and Magnetic Instabilities and Hysteresis in Heuslers by Density Functional Theory Calculations (Phys. Status Solidi B 2/2018). Physica Status Solidi (B): Basic Research, 2018, 255, 1870108. | 0.7 | 2 |
| 79 | Firstâ€Principles Characterization of Equilibrium Vacancy Concentration in Metamagnetic Shape Memory Alloys: An Example of Ni‹sub›2‹/sub›MnGa. Physica Status Solidi (B): Basic Research, 2018, 255, 1700523. | 0.7 | 6 |
| 80 | Out-of-plane ordering in quaternary MAX alloys: an alloy theoretic perspective. Materials Research Letters, 2018, 6, 1-12. | 4.1 | 5 |
| 81 | Probing Structural and Magnetic Instabilities and Hysteresis in Heuslers by Density Functional Theory Calculations. Physica Status Solidi (B): Basic Research, 2018, 255, 1700296. | 0.7 | 11 |
| 82 | On the microstructural origins of martensitic transformation arrest in a NiCoMnIn magnetic shape memory alloy. Acta Materialia, 2018, 142, 95-106. | 3.8 | 67 |
| 83 | Multi-Information Source Fusion and Optimization to Realize ICME: Application to Dual-Phase Materials. Journal of Mechanical Design, Transactions of the ASME, 2018, 140, . | 1.7 | 32 |
| 84 | Influence of deposition temperature on the properties of sputtered films grown from a Cu2O CdO TeO2 composite target: Electronic properties of CdTe2O5. Superlattices and Microstructures, 2018, 123, 403-413. | 1.4 | 1 |
| 85 | On the printability and transformation behavior of nickel-titanium shape memory alloys fabricated using laser powder-bed fusion additive manufacturing. Journal of Manufacturing Processes, 2018, 35, 672-680. | 2.8 | 75 |
| 86 | Multi-objective Bayesian materials discovery: Application on the discovery of precipitation strengthened NiTi shape memory alloys through micromechanical modeling. Materials and Design, 2018, 160, 810-827. | 3.3 | 83 |
| 87 | On the interfacial phase growth and vacancy evolution during accelerated electromigration in Cu/Sn/Cu microjoints. Acta Materialia, 2018, 160, 185-198. | 3.8 | 35 |
| 88 | Interdisciplinary Research on Designing Engineering Material Systems: Results From a National Science Foundation Workshop. Journal of Mechanical Design, Transactions of the ASME, 2018, 140, . | 1.7 | 11 |
| 89 | Multivariate Calibration and Experimental Validation of a 3D Finite Element Thermal Model for Laser Powder Bed Fusion Metal Additive Manufacturing. Integrating Materials and Manufacturing Innovation, 2018, 7, 116-135. | 1.2 | 36 |
| 90 | Computational Design of Gradient Paths in Additively Manufactured Functionally Graded Materials. Journal of Mechanical Design, Transactions of the ASME, 2018, 140, . | 1.7 | 19 |

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| 92 | Phase transformations in equiatomic CuZr shape memory thin films analyzed by differential nanocalorimetry. Acta Materialia, 2018, 159, 320-331. | 3.8 | 15 |
| 93 | Uncertainty Propagation Analysis of Computational Models in Laser Powder Bed Fusion Additive Manufacturing Using Polynomial Chaos Expansions. Journal of Manufacturing Science and Engineering, Transactions of the ASME, 2018, 140, . | 1.3 | 41 |
| 94 | Strain-induced suppression of the miscibility gap in nanostructured Mg<sub>2</sub>Siâ€“Mg<sub>2</sub>Sn solid solutions. Journal of Materials Chemistry A, 2018, 6, 17559-17570. | 5.2 | 30 |
| 95 | Glassy Phonon Heralds a Strain Glass State in a Shape Memory Alloy. Physical Review Letters, 2018, 120, 245701. | 2.9 | 24 |
| 96 | Nucleation-controlled hysteresis in unstrained hydrothermal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">V</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> particles. Physical Review Materials, 2018, 2, . | 0.9 | 10 |
| 97 | Autonomous efficient experiment design for materials discovery with Bayesian model averaging. Physical Review Materials, 2018, 2, . | 0.9 | 58 |
| 98 | A Constraint Satisfaction Algorithm for the Generalized Inverse Phase Stability Problem. Journal of Mechanical Design, Transactions of the ASME, 2017, 139, . | 1.7 | 9 |
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| 100 | Real-time atomistic observation of structural phase transformations in individual hafnia nanorods. Nature Communications, 2017, 8, 15316. | 5.8 | 59 |
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| 102 | Spatial Control of Functional Response in 4D-Printed Active Metallic Structures. Scientific Reports, 2017, 7, 46707. | 1.6 | 109 |
| 103 | A data-driven machine learning approach to predicting stacking faulting energy in austenitic steels. Journal of Materials Science, 2017, 52, 11048-11076. | 1.7 | 35 |
| 104 | Looking Outwards from the â€œCentral Scienceâ€: An Interdisciplinary Perspective on Graduate Education in Materials Chemistry. ACS Symposium Series, 2017, , 65-89. | 0.5 | 3 |
| 105 | On the stochastic phase stability of Ti2AlC-Cr2AlC. Scientific Reports, 2017, 7, 5138. | 1.6 | 16 |
| 106 | A Sensory Material Approach for Reducing Variability in Additively Manufactured Metal Parts. Scientific Reports, 2017, 7, 3604. | 1.6 | 55 |
| 107 | Does aluminum play well with others? Intrinsic Al-A alloying behavior in 211/312 MAX phases. Materials Research Letters, 2017, 5, 170-178. | 4.1 | 20 |
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| 110 | Revisiting thermodynamics and kinetic diffusivities of uraniumâ€“niobium with Bayesian uncertainty analysis. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2016, 55, 219-230. | 0.7 | 46 |
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| 112 | High-throughput combinatorial study of the effect of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>M</mml:mi></mml:math>site alloying on the solid solution behavior of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>M</mml:mi><mml:mn>2</mml:mn></mml:n phases. Physical Review B, 2016, 94, . | 1.1 | 38 |
| 113 | Phase Field Modeling of Joint Formation During Isothermal Solidification in 3DIC Micro Packaging. Journal of Phase Equilibria and Diffusion, 2016, 37, 469-480. | 0.5 | 9 |
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| 115 | The Inverse Phase Stability Problem as a Constraint Satisfaction Problem: Application to Materials Design. Jom, 2016, 68, 1385-1395. | 0.9 | 8 |
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| 117 | Tailored thermal expansion alloys. Acta Materialia, 2016, 102, 333-341. | 3.8 | 92 |
| 118 | Describing the deformation behaviour of TRIP and dual phase steels employing an irreversible thermodynamics formulation. Materials Science and Technology, 2015, 31, 1658-1663. | 0.8 | 5 |
| 119 | Stability analysis of the martensitic phase transformation in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Co</mml:mi><mml:mn>2</mml:mn></mml:m alloy. Physical Review B, 2015, 92, . | 1.1 | 11 |
| 120 | Lattice vibrations boost demagnetization entropy in a shape-memory alloy. Physical Review B, 2015, 92, . | 1.1 | 19 |
| 121 | Computational Thermodynamics and Kinetics-Based ICME Framework for High-Temperature Shape Memory Alloys. Shape Memory and Superelasticity, 2015, 1, 429-449. | 1.1 | 1 |
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| 123 | Metal cluster-deposited graphene as an adsorptive material for m-xylene. New Journal of Chemistry, 2015, 39, 9650-9658. | 1.4 | 19 |
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| 125 | Constraint Satisfaction Approach to the Design of Multi-Component, Multi-Phase Alloys. , 2014, , . | | 2 |
| 126 | Effect of Student-Led Undergraduate Research Experience on Learning and Attitudes --A Practice in An Introductory Materials Science Course. Materials Research Society Symposia Proceedings, 2014, 1657, 38. | 0.1 | 0 |

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| 130 | First-principles calculation of the instability leading to giant inverse magnetocaloric effects. Physical Review B, 2014, 89, . | 1.1 | 73 |
| 131 | Confinement Effects on Evolution of Intermetallic Compounds During Metallurgical Joint Formation. Journal of Electronic Materials, 2014, 43, 2510-2520. | 1.0 | 5 |
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| 137 | Commentary: Recent Advances in Ab Initio Thermodynamics of Materials. Jom, 2013, 65, 1499-1500. | 0.9 | 0 |
| 138 | Phase constitution effect on the ductility of low alloy multiphase transformation induced plasticity steels. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2013, 569, 137-143. | 2.6 | 25 |
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| 154 | A Firstâ€Principles Investigation of the Compositional Dependent Properties of Magnetic Shape Memory Heusler Alloys. Advanced Engineering Materials, 2012, 14, 530-546. | 1.6 | 54 |
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