# Adri van Duin

## List of Publications by Year in Descending Order



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| 349 papers | 20,902 citations | 70 h-index | 135 g-index |
| 370 ext. papers | 24,633 ext. citations | 5.5 avg, IF | 7.28 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 349 | Development of a Charge-Implicit ReaxFF for C/H/O Systems.. *Journal of Physical Chemistry Letters*, **2022**, 13, 628-633 | 6.4 | 1 |
| 348 | ReaxFF Force Field Development for Gas-Phase hBN Nanostructure Synthesis.. *Journal of Physical Chemistry A*, **2022**, | 2.8 | 1 |
| 347 | Atomic-scale probing of defect-assisted Ga intercalation through graphene using ReaxFF molecular dynamics simulations. *Carbon*, **2022**, 190, 276-290 | 10.4 | 3 |
| 346 | A reactive force field molecular dynamics study on the inception mechanism of titanium tetraisopropoxide (TTIP) conversion to titanium clusters. *Chemical Engineering Science*, **2022**, 252, 117496 | 4.4 | 1 |
| 345 | A ReaxFF Molecular Dynamics Study of Hydrogen Diffusion in Ruthenium-The Role of Grain Boundaries.. *Journal of Physical Chemistry C*, **2022**, 126, 5950-5959 | 3.8 | 1 |
| 344 | A reactive molecular dynamics study of bi-modal particle size distribution in binder-jetting additive manufacturing using stainless-steel powders.. *Physical Chemistry Chemical Physics*, **2022**, 24, 11603-11615 | 3.6 | |
| 343 | Molecular Dynamics Modeling of Interfacial Interactions between Flattened Carbon Nanotubes and Amorphous Carbon: Implications for Ultra-Lightweight Composites.. *ACS Applied Nano Materials*, **2022**, 5, 5915-5924 | 5.6 | 2 |
| 342 | Using C-DFT to develop an e-ReaxFF force field for acetophenone radical anion. *Journal of Chemical Physics*, **2021**, 155, 214104 | 3.9 | 0 |
| 341 | Understanding physical chemistry of BaSrTiO using ReaxFF molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2021**, 23, 25056-25062 | 3.6 | |
| 340 | Oxygen Vacancy Injection as a Pathway to Enhancing Electromechanical Response in Ferroelectrics. *Advanced Materials*, **2021**, e2106426 | 24 | 1 |
| 339 | Machine Learning-Assisted Hybrid ReaxFF Simulations. *Journal of Chemical Theory and Computation*, **2021**, 17, 6705-6712 | 6.4 | 1 |
| 338 | Mechanistic study of pH effect on organic solvent nanofiltration using carboxylated covalent organic framework as a modeling and experimental platform. *Separation and Purification Technology*, **2021**, 282, 120028 | 8.3 | 1 |
| 337 | Formation of metal vacancy arrays in coalesced WS2 monolayer films. *2D Materials*, **2021**, 8, 011003 | 5.9 | 7 |
| 336 | Unimolecular Pyrolysis Mechanism of Thiophene and Furan: An Ab Initio Comparative Study. *Energy & Fuels*, **2021**, 35, 7819-7832 | 4.1 | 1 |
| 335 | Interfacial Reactivity and Speciation Emerging from Na-Montmorillonite Interactions with Water and Formic Acid at 200 °C: Insights from Reactive Molecular Dynamics Simulations, Infrared Spectroscopy, and X-ray Scattering Measurements. *ACS Earth and Space Chemistry*, **2021**, 5, 1006-1019 | 3.2 | 2 |
| 334 | Subsurface structural change of silica upon nanoscale physical contact: Chemical plasticity beyond topographic elasticity. *Acta Materialia*, **2021**, 208, 116694 | 8.4 | 10 |
| 333 | Dynamics of the Chemically Driven Densification of Barium Titanate Using Molten Hydroxides. *Nano Letters*, **2021**, 21, 3451-3457 | 11.5 | 7 |

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| 332 | INDEEDopt: a deep learning-based ReaxFF parameterization framework. *Npj Computational Materials*, **2021**, 7, | 10.9 | 6 |
| 331 | Recent Advances for Improving the Accuracy, Transferability, and Efficiency of Reactive Force Fields. *Journal of Chemical Theory and Computation*, **2021**, 17, 3237-3251 | 6.4 | 17 |
| 330 | Development and Applications of ReaxFF Reactive Force Fields for Group-III Gas-Phase Precursors and Surface Reactions with Graphene in Metal Organic Chemical Vapor Deposition Synthesis. *Journal of Physical Chemistry C*, **2021**, 125, 10747-10758 | 3.8 | 3 |
| 329 | Atomistic Insights Into the Degradation of Inorganic Halide Perovskite CsPbI: A Reactive Force Field Molecular Dynamics Study. *Journal of Physical Chemistry Letters*, **2021**, 12, 5519-5525 | 6.4 | 7 |
| 328 | Nanomechanical investigation of the interplay between pore morphology and crack orientation of amorphous silica. *Engineering Fracture Mechanics*, **2021**, 250, 107749 | 4.2 | 1 |
| 327 | Atomistic Insights on the Full Operation Cycle of a HfO-Based Resistive Random Access Memory Cell from Molecular Dynamics. *ACS Nano*, **2021**, 15, 12945-12954 | 16.7 | 5 |
| 326 | Illuminating Invisible Grain Boundaries in Coalesced Single-Orientation WS Monolayer Films. *Nano Letters*, **2021**, 21, 6487-6495 | 11.5 | 7 |
| 325 | Effects of pressure and velocity on the interface friction behavior of diamond utilizing ReaxFF simulations. *International Journal of Mechanical Sciences*, **2021**, 191, 106096 | 5.5 | 11 |
| 324 | An environmental-friendly process for dissociating toxic substances and recovering valuable components from spent carbon cathode. *Journal of Hazardous Materials*, **2021**, 404, 124120 | 12.8 | 8 |
| 323 | Low-temperature carbonization of polyacrylonitrile/graphene carbon fibers: A combined ReaxFF molecular dynamics and experimental study. *Carbon*, **2021**, 174, 345-356 | 10.4 | 20 |
| 322 | Atomistic Mechanisms of Thermal Transformation in a Zr-Metal Organic Framework, MIL-140C. *Journal of Physical Chemistry Letters*, **2021**, 12, 177-184 | 6.4 | 3 |
| 321 | CLAIMED: A CLAssification-Incorporated Minimum Energy Design to Explore a Multivariate Response Surface With Feasibility Constraints. *IEEE Transactions on Automation Science and Engineering*, **2021**, 1-12 | 4.9 | |
| 320 | ReaxFF reactive molecular dynamics simulations to study the interfacial dynamics between defective h-BN nanosheets and water nanodroplets. *Physical Chemistry Chemical Physics*, **2021**, 23, 10822-10834 | 3.6 | 23 |
| 319 | Wafer-Scale Lateral Self-Assembly of Mosaic TiCT MXene Monolayer Films. *ACS Nano*, **2021**, 15, 625-636 | 16.7 | 20 |
| 318 | Atomistic-Scale Simulations on Graphene Bending Near a Copper Surface. *Catalysts*, **2021**, 11, 208 | 4 | 2 |
| 317 | Interfacial Bonding Controls Friction in Diamond Rock Contacts. *Journal of Physical Chemistry C*, **2021**, 125, 18395-18408 | 3.8 | 1 |
| 316 | ReaxFF molecular dynamics study on pyrolysis of bicyclic compounds for aviation fuel. *Fuel*, **2021**, 297, 120724 | 7.1 | 10 |
| 315 | Effects of interlayer confinement and hydration on capacitive charge storage in birnessite. *Nature Materials*, **2021**, 20, 1689-1694 | 27 | 21 |

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| 314 | A ReaxFF Force Field for 2D-WS2 and Its Interaction with Sapphire. *Journal of Physical Chemistry C*, **2021**, 125, 17950-17961 | 3.8 | 3 |
| 313 | Molecular Interactions and Layer Stacking Dictate Covalent Organic Framework Effective Pore Size. *ACS Applied Materials & Interfaces*, **2021**, 13, 42164-42175 | 9.5 | 2 |
| 312 | Development of the ReaxFF Reactive Force Field for Cu/Si Systems with Application to Copper Cluster Formation during Cu Diffusion Inside Silicon. *Journal of Physical Chemistry C*, **2021**, 125, 19455-19466 | 3.8 | 1 |
| 311 | Influence mechanism of Nano-Fe2O3 on amorphous carbon graphitisation in molecular view via ReaxFF MD simulation. *Molecular Simulation*, **2021**, 47, 1241-1249 | 2 | 0 |
| 310 | Tunable 2D Group-III Metal Alloys. *Advanced Materials*, **2021**, 33, e2104265 | 24 | 6 |
| 309 | Impact of three-body interactions in a ReaxFF force field for Ni and Cr transition metals and their alloys on the prediction of thermal and mechanical properties. *Computational Materials Science*, **2021**, 197, 110602 | 3.2 | 1 |
| 308 | Investigating the Accuracy of Water Models through the Van Hove Correlation Function. *Journal of Chemical Theory and Computation*, **2021**, 17, 5992-6005 | 6.4 | 3 |
| 307 | Theoretical modeling of edge-controlled growth kinetics and structural engineering of 2D-MoSe2. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **2021**, 271, 115263 | 3.1 | 3 |
| 306 | Molecular dynamics study of melting, diffusion, and sintering of cementite chromia core□shell particles. *Computational Materials Science*, **2021**, 199, 110721 | 3.2 | 1 |
| 305 | Atomistic-scale insight into the polyethylene electrical breakdown: An eReaxFF molecular dynamics study. *Journal of Chemical Physics*, **2021**, 154, 024904 | 3.9 | 3 |
| 304 | Experimental and computational investigations of ethane and ethylene kinetics with copper oxide particles for Chemical Looping Combustion. *Proceedings of the Combustion Institute*, **2021**, 38, 5249-5257 | 5.9 | 1 |
| 303 | Modeling for Structural Engineering and Synthesis of Two-Dimensional WSe2 Using a Newly Developed ReaxFF Reactive Force Field. *Journal of Physical Chemistry C*, **2020**, 124, 28285-28297 | 3.8 | 10 |
| 302 | Detoxification and Recovery of Spent Carbon Cathodes via NaOH□Na2CO3 Binary Molten Salt Roasting□Water Leaching: Toward a Circular Economy for Hazardous Solid Waste from Aluminum Electrolysis. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 16912-16923 | 8.3 | 4 |
| 301 | Reactive Molecular Dynamics Simulations and Quantum Chemistry Calculations To Investigate Soot-Relevant Reaction Pathways for Hexylamine Isomers. *Journal of Physical Chemistry A*, **2020**, 124, 4290-4304 | 2.8 | 8 |
| 300 | Investigation into the Atomistic Scale Mechanisms Responsible for the Enhanced Dielectric Response in the Interfacial Region of Polymer Nanocomposites. *Journal of Physical Chemistry C*, **2020**, 124, 11558-11563 | 3.8 | 7 |
| 299 | Development of a Reactive Force Field for Simulations on the Catalytic Conversion of C/H/O Molecules on Cu-Metal and Cu-Oxide Surfaces and Application to Cu/CuO-Based Chemical Looping. *Journal of Physical Chemistry C*, **2020**, 124, 12512-12520 | 3.8 | 7 |
| 298 | Lithium-electrolyte solvation and reaction in the electrolyte of a lithium ion battery: A ReaxFF reactive force field study. *Journal of Chemical Physics*, **2020**, 152, 184301 | 3.9 | 15 |
| 297 | ReaxFF molecular dynamics simulations of electrolyte-water systems at supercritical temperature. *Journal of Chemical Physics*, **2020**, 152, 204502 | 3.9 | 5 |

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| 296 | Full-Scale Ab Initio Simulation of Magic-Angle-Spinning Dynamic Nuclear Polarization. *Journal of Physical Chemistry Letters*, **2020**, 11, 5655-5660 | 6.4 | 14 |
| 295 | Reactive molecular dynamics simulation for isotope-exchange reactions in H/D systems: ReaxFF development. *Journal of Chemical Physics*, **2020**, 152, 224111 | 3.9 | 2 |
| 294 | Simulations of the Biodegradation of Citrate-Based Polymers for Artificial Scaffolds Using Accelerated Reactive Molecular Dynamics. *Journal of Physical Chemistry B*, **2020**, 124, 5311-5322 | 3.4 | 6 |
| 293 | Multiscale computational understanding and growth of 2D materials: a review. *Npj Computational Materials*, **2020**, 6, | 10.9 | 49 |
| 292 | Atomically thin half-van der Waals metals enabled by confinement heteroepitaxy. *Nature Materials*, **2020**, 19, 637-643 | 27 | 53 |
| 291 | ReaxFF Simulations of Laser-Induced Graphene (LIG) Formation for Multifunctional Polymer Nanocomposites. *ACS Applied Nano Materials*, **2020**, 3, 1881-1890 | 5.6 | 30 |
| 290 | Reactive Molecular Dynamics Study of Hierarchical Tribochemical Lubricant Films at Elevated Temperatures. *ACS Applied Nano Materials*, **2020**, 3, 2687-2704 | 5.6 | 5 |
| 289 | Timescale prediction of complex multi-barrier pathways using flux sampling molecular dynamics and 1D kinetic integration: Application to cellulose dehydration. *Journal of Chemical Physics*, **2020**, 152, 024123 | 3.9 | 4 |
| 288 | Searching for correlations between vibrational spectral features and structural parameters of silicate glass network. *Journal of the American Ceramic Society*, **2020**, 103, 3575-3589 | 3.8 | 16 |
| 287 | Simulating the Geological Fate of Terrestrial Organic Matter: Lignin vs Cellulose. *Energy & Fuels*, **2020**, 34, 1537-1547 | 4.1 | 6 |
| 286 | Atomistic understanding of surface wear process of sodium silicate glass in dry versus humid environments. *Journal of the American Ceramic Society*, **2020**, 103, 3060-3069 | 3.8 | 18 |
| 285 | Graphene reinforced carbon fibers. *Science Advances*, **2020**, 6, eaaz4191 | 14.3 | 40 |
| 284 | Friction-induced subsurface densification of glass at contact stress far below indentation damage threshold. *Acta Materialia*, **2020**, 189, 166-173 | 8.4 | 20 |
| 283 | Influence of acid leaching surface treatment on indentation cracking of soda lime silicate glass. *Journal of Non-Crystalline Solids*, **2020**, 543, 120144 | 3.9 | 7 |
| 282 | ReaxFF molecular dynamics simulations on the structure and dynamics of electrolyte water systems at ambient temperature. *Computational Materials Science*, **2020**, 172, 109349 | 3.2 | 9 |
| 281 | Understanding the chemistry of cation leaching in illite/water interfacial system using reactive molecular dynamics simulations and hydrothermal experiments. *Acta Materialia*, **2020**, 186, 564-574 | 8.4 | 6 |
| 280 | High Peel Strength and Flexible Aligned Carbon Nanotubes/Etched Al Foil Composites with Boosted Supercapacitor and Thermal Dissipation Performances. *Industrial & Engineering Chemistry Research*, **2020**, 59, 1549-1558 | 3.9 | 2 |
| 279 | Converting PBO fibers into carbon fibers by ultrafast carbonization. *Carbon*, **2020**, 159, 432-442 | 10.4 | 9 |

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| 278 | Numerical simulations of yield-based sooting tendencies of aromatic fuels using ReaxFF molecular dynamics. *Fuel*, **2020**, 262, 116545 | 7.1 | 17 |
| 277 | Predicting cost-effective carbon fiber precursors: Unraveling the functionalities of oxygen and nitrogen-containing groups during carbonization from ReaxFF simulations. *Carbon*, **2020**, 159, 25-36 | 10.4 | 23 |
| 276 | Elucidating Thermally Induced Structural and Chemical Transformations in Kaolinite Using Reactive Molecular Dynamics Simulations and X-ray Scattering Measurements. *Chemistry of Materials*, **2020**, 32, 651-662 | 9.6 | 9 |
| 275 | Comparing hydrothermal sintering and cold sintering process: Mechanisms, microstructure, kinetics and chemistry. *Journal of the European Ceramic Society*, **2020**, 40, 1312-1324 | 6 | 28 |
| 274 | Optimization of the Reax force field for the lithium-oxygen system using a high fidelity charge model. *Journal of Chemical Physics*, **2020**, 153, 084107 | 3.9 | 5 |
| 273 | ReaxFF-based molecular dynamics study of bio-derived polycyclic alkanes as potential alternative jet fuels. *Fuel*, **2020**, 279, 118548 | 7.1 | 20 |
| 272 | Roadmap for densification in cold sintering: Chemical pathways. *Open Ceramics*, **2020**, 2, 100019 | 3.3 | 12 |
| 271 | Stable metal anodes enabled by a labile organic molecule bonded to a reduced graphene oxide aerogel. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 30135-30141 | 11.5 | 6 |
| 270 | Two-dimensional hybrid organic–inorganic perovskites as emergent ferroelectric materials. *Journal of Applied Physics*, **2020**, 128, 060906 | 2.5 | 13 |
| 269 | ReaxFF/AMBER-A Framework for Hybrid Reactive/Nonreactive Force Field Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2020**, 16, 7645-7654 | 6.4 | 5 |
| 268 | Enhanced Fuel Decomposition in the Presence of Colloidal Functionalized Graphene Sheet-Supported Platinum Nanoparticles. *ACS Applied Energy Materials*, **2020**, 3, 7637-7648 | 6.1 | 2 |
| 267 | ReaxFF Reactive Force Field Study of Polymerization of a Polymer Matrix in a Carbon Nanotube-Composite System. *Journal of Physical Chemistry C*, **2020**, 124, 20488-20497 | 3.8 | 12 |
| 266 | Atomistic-Scale Simulations of the Graphene Growth on a Silicon Carbide Substrate Using Thermal Decomposition and Chemical Vapor Deposition. *Chemistry of Materials*, **2020**, 32, 8306-8317 | 9.6 | 11 |
| 265 | Development and initial applications of an e-ReaxFF description of Ag nanoclusters. *Journal of Chemical Physics*, **2020**, 153, 104106 | 3.9 | 9 |
| 264 | Structure and Dynamics of Aqueous Electrolytes Confined in 2D-TiO/TiCT MXene Heterostructures. *ACS Applied Materials & Interfaces*, **2020**, 12, 58378-58389 | 9.5 | 4 |
| 263 | Structural features of sodium silicate glasses from reactive force field-based molecular dynamics simulations. *Journal of the American Ceramic Society*, **2020**, 103, 1600-1614 | 3.8 | 15 |
| 262 | Reductive Gaseous (H2/NH3) Desulfurization and Gasification of High-Sulfur Petroleum Coke via Reactive Force Field Molecular Dynamics Simulations. *Energy & Fuels*, **2019**, 33, 8065-8075 | 4.1 | 7 |
| 261 | A ReaxFF molecular dynamics study of molecular-level interactions during binder jetting 3D-printing. *Physical Chemistry Chemical Physics*, **2019**, 21, 21517-21529 | 3.6 | 5 |

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| 260 | Topological Control of Water Reactivity on Glass Surfaces: Evidence of a Chemically Stable Intermediate Phase. *Journal of Physical Chemistry Letters*, **2019**, 10, 3955-3960 | 6.4 | 3 |
| 259 | Reactive Force Field for Simulations of the Pyrolysis of Polysiloxanes into Silicon Oxycarbide Ceramics. *Journal of Physical Chemistry C*, **2019**, 123, 16804-16812 | 3.8 | 10 |
| 258 | Reactive Molecular Dynamics Simulations of the Atomic Oxygen Impact on Epoxies with Different Chemistries. *Journal of Physical Chemistry C*, **2019**, 123, 15145-15156 | 3.8 | 12 |
| 257 | Surface Reactivity and Leaching of a Sodium Silicate Glass under an Aqueous Environment: A ReaxFF Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2019**, 123, 15606-15617 | 3.8 | 32 |
| 256 | Atomistic Scale Analysis of the Carbonization Process for C/H/O/N-Based Polymers with the ReaxFF Reactive Force Field. *Journal of Physical Chemistry B*, **2019**, 123, 5357-5367 | 3.4 | 53 |
| 255 | Statistical Analysis of Tri-Cresyl Phosphate Conversion on an Iron Oxide Surface Using Reactive Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2019**, | 3.8 | 7 |
| 254 | Atomistic insights on the influence of pre-oxide shell layer and size on the compressive mechanical properties of nickel nanowires. *Journal of Applied Physics*, **2019**, 125, 165102 | 2.5 | 4 |
| 253 | Development of the ReaxFF Reactive Force Field for Inherent Point Defects in the Si/Silica System. *Journal of Physical Chemistry A*, **2019**, 123, 4303-4313 | 2.8 | 10 |
| 252 | Mechanical size effects of amorphous polymer-derived ceramics at the nanoscale: experiments and ReaxFF simulations. *Nanoscale*, **2019**, 11, 7447-7456 | 7.7 | 13 |
| 251 | Predicting the preferred morphology of hexagonal boron nitride domain structure on nickel from ReaxFF-based molecular dynamics simulations. *Nanoscale*, **2019**, 11, 5607-5616 | 7.7 | 12 |
| 250 | Application of ReaxFF-Reactive Molecular Dynamics and Continuum Methods in High-Temperature/Pressure Pyrolysis of Fuel Mixtures. *Challenges and Advances in Computational Chemistry and Physics*, **2019**, 161-185 | 0.7 | 2 |
| 249 | Hydroxide transport and chemical degradation in anion exchange membranes: a combined reactive and non-reactive molecular simulation study. *Journal of Materials Chemistry A*, **2019**, 7, 5442-5452 | 13 | 28 |
| 248 | Pyrolysis of binary fuel mixtures at supercritical conditions: A ReaxFF molecular dynamics study. *Fuel*, **2019**, 235, 194-207 | 7.1 | 42 |
| 247 | Effects of water on the mechanical properties of silica glass using molecular dynamics. *Acta Materialia*, **2019**, 178, 36-44 | 8.4 | 12 |
| 246 | Multiply accelerated ReaxFF molecular dynamics: coupling parallel replica dynamics with collective variable hyper dynamics. *Molecular Simulation*, **2019**, 45, 1265-1272 | 2 | 5 |
| 245 | Water-Mediated Surface Diffusion Mechanism Enables the Cold Sintering Process: A Combined Computational and Experimental Study. *Angewandte Chemie*, **2019**, 131, 12550-12554 | 3.6 | 8 |
| 244 | Formation of AlFx Gaseous Phases during High Temperature Etching: A Reactive Force Field Based Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2019**, 123, 16823-16835 | 3.8 | 2 |
| 243 | Understanding the influence of defects and surface chemistry on ferroelectric switching: a ReaxFF investigation of BaTiO. *Physical Chemistry Chemical Physics*, **2019**, 21, 18240-18249 | 3.6 | 28 |

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| 242 | Water-Mediated Surface Diffusion Mechanism Enables the Cold Sintering Process: A Combined Computational and Experimental Study. *Angewandte Chemie - International Edition*, **2019**, 58, 12420-12424 | 16.4 | 22 |
| 241 | ReaxFF MD simulations of petroleum coke CO2 gasification examining the S/N removal mechanisms and CO/CO2 reactivity. *Fuel*, **2019**, 257, 116051 | 7.1 | 8 |
| 240 | Atomistic-scale insights into the crosslinking of polyethylene induced by peroxides. *Polymer*, **2019**, 183, 121901 | 3.9 | 25 |
| 239 | Multi-scale modeling of gas-phase reactions in metal-organic chemical vapor deposition growth of WSe2. *Journal of Crystal Growth*, **2019**, 527, 125247 | 1.6 | 25 |
| 238 | Atomistic Insights into Cu Chemical Mechanical Polishing Mechanism in Aqueous Hydrogen Peroxide and Glycine: ReaxFF Reactive Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2019**, 123, 26467-26474 | 3.8 | 14 |
| 237 | Unveiling Carbon Ring Structure Formation Mechanisms in Polyacrylonitrile-Derived Carbon Fibers. *ACS Applied Materials & Interfaces*, **2019**, 11, 42288-42297 | 9.5 | 15 |
| 236 | How to characterize interfacial load transfer in spiral carbon-based nanostructure-reinforced nanocomposites: is this a geometry-dependent process?. *Physical Chemistry Chemical Physics*, **2019**, 21, 23880-23892 | 3.6 | 6 |
| 235 | ReaxFF Parameter Optimization with Monte-Carlo and Evolutionary Algorithms: Guidelines and Insights. *Journal of Chemical Theory and Computation*, **2019**, 15, 6799-6812 | 6.4 | 35 |
| 234 | Molecular Dynamics Simulations of MXenes: Ab Initio, Reactive, and Non-reactive Empirical Force Fields **2019**, 137-157 | | 1 |
| 233 | Development of the ReaxFF Methodology for Electrolyte-Water Systems. *Journal of Physical Chemistry A*, **2019**, 123, 2125-2141 | 2.8 | 19 |
| 232 | Modification of activated carbon with a silane coupling agent under ultrasonic conditions for the advanced treatment of wastewater with dressing chemicals. *Coloration Technology*, **2019**, 135, 67-76 | 2 | 5 |
| 231 | Development of a ReaxFF Reactive Force Field for Interstitial Oxygen in Germanium and Its Application to GeO2/Ge Interfaces. *Journal of Physical Chemistry C*, **2019**, 123, 1208-1218 | 3.8 | 8 |
| 230 | A roadmap for electronic grade 2D materials. *2D Materials*, **2019**, 6, 022001 | 5.9 | 133 |
| 229 | Cathodic Corrosion at the Bismuth/Ionic Liquid Electrolyte Interface under Conditions for CO2 Reduction. *Chemistry of Materials*, **2018**, 30, 2362-2373 | 9.6 | 26 |
| 228 | Improvement of the ReaxFF Description for Functionalized Hydrocarbon/Water Weak Interactions in the Condensed Phase. *Journal of Physical Chemistry B*, **2018**, 122, 4083-4092 | 3.4 | 50 |
| 227 | Phase transitions of ordered ice in graphene nanocapillaries and carbon nanotubes. *Scientific Reports*, **2018**, 8, 3851 | 4.9 | 33 |
| 226 | A first-principles study of stability of surface confined mixed metal oxides with corundum structure (FeO, CrO, VO). *Physical Chemistry Chemical Physics*, **2018**, 20, 7073-7081 | 3.6 | 6 |
| 225 | Grotthuss versus Vehicular Transport of Hydroxide in Anion-Exchange Membranes: Insight from Combined Reactive and Nonreactive Molecular Simulations. *Journal of Physical Chemistry Letters*, **2018**, 9, 825-829 | 6.4 | 45 |

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| 224 | Optimization of purification treatment of spent cathode carbon from aluminum electrolysis using response surface methodology (RSM). *Asia-Pacific Journal of Chemical Engineering*, **2018**, 13, e2164 | 1.3 | 3 |
| 223 | Structural features of Qingdao petroleum coke from HRTEM lattice fringes: Distributions of length, orientation, stacking, curvature, and a large-scale image-guided 3D atomistic representation. *Carbon*, **2018**, 129, 790-802 | 10.4 | 60 |
| 222 | Development of a Charge-Implicit ReaxFF Potential for Hydrocarbon Systems. *Journal of Physical Chemistry Letters*, **2018**, 9, 359-363 | 6.4 | 13 |
| 221 | Do Nickel and Iron catalyst nanoparticles affect the mechanical strength of carbon nanotubes?. *Extreme Mechanics Letters*, **2018**, 20, 29-37 | 3.9 | 8 |
| 220 | Carbon structure and the resulting graphitizability upon oxygen evolution. *Carbon*, **2018**, 135, 171-179 | 10.4 | 19 |
| 219 | ReaxFF molecular dynamics simulation of intermolecular structure formation in acetic acid-water mixtures at elevated temperatures and pressures. *Journal of Chemical Physics*, **2018**, 148, 164506 | 3.9 | 18 |
| 218 | Development of a ReaxFF Force Field for Cu/S/C/H and Reactive MD Simulations of Methyl Thiolate Decomposition on Cu (100). *Journal of Physical Chemistry B*, **2018**, 122, 888-896 | 3.4 | 14 |
| 217 | Benchmark of ReaxFF force field for subcritical and supercritical water. *Journal of Chemical Physics*, **2018**, 148, 234503 | 3.9 | 23 |
| 216 | Complexity of Intercalation in MXenes: Destabilization of Urea by Two-Dimensional Titanium Carbide. *Journal of the American Chemical Society*, **2018**, 140, 10305-10314 | 16.4 | 58 |
| 215 | Theoretical prediction electronic properties of Group-IV diamond nanothreads. *AIP Advances*, **2018**, 8, 075107 | 1.5 | 5 |
| 214 | Accelerated ReaxFF Simulations for Describing the Reactive Cross-Linking of Polymers. *Journal of Physical Chemistry A*, **2018**, 122, 6633-6642 | 2.8 | 52 |
| 213 | Defect Design of Two-Dimensional MoS2 Structures by Using a Graphene Layer and Potato Stamp Concept. *Journal of Physical Chemistry C*, **2018**, 122, 11911-11917 | 3.8 | 11 |
| 212 | Development of a ReaxFF Reactive Force Field for NaSiOx/Water Systems and Its Application to Sodium and Proton Self-Diffusion. *Journal of Physical Chemistry C*, **2018**, 122, 19613-19624 | 3.8 | 41 |
| 211 | Development of a ReaxFF reactive force field for lithium ion conducting solid electrolyte LiAlTi(PO) (LATP). *Physical Chemistry Chemical Physics*, **2018**, 20, 22134-22147 | 3.6 | 14 |
| 210 | Oxyhydroxide of metallic nanowires in a molecular HO and HO environment and their effects on mechanical properties. *Physical Chemistry Chemical Physics*, **2018**, 20, 17289-17303 | 3.6 | 14 |
| 209 | Hydrogenation and defect formation control the strength and ductility of MoS2 nanosheets: Reactive molecular dynamics simulation. *Extreme Mechanics Letters*, **2018**, 22, 157-164 | 3.9 | 13 |
| 208 | In situ atomistic insight into the growth mechanisms of single layer 2D transition metal carbides. *Nature Communications*, **2018**, 9, 2266 | 17.4 | 89 |
| 207 | A comparative study on the oxidation of two-dimensional Ti3C2 MXene structures in different environments. *Journal of Materials Chemistry A*, **2018**, 6, 12733-12743 | 13 | 124 |

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| 206 | Raman spectroscopy revealing noble gas adsorption on single-walled carbon nanotube bundles. *Carbon*, **2018**, 127, 312-319 | 10.4 | 15 |
| 205 | Co-treatment of spent cathode carbon in caustic and acid leaching process under ultrasonic assisted for preparation of SiC. *Ultrasonics Sonochemistry*, **2018**, 41, 608-618 | 8.9 | 27 |
| 204 | Multiscale Modeling of Structure, Transport and Reactivity in Alkaline Fuel Cell Membranes: Combined Coarse-Grained, Atomistic and Reactive Molecular Dynamics Simulations. *Polymers*, **2018** , 10, | 4.5 | 16 |
| 203 | Prediction of the Glass Transition Temperatures of Zeolitic Imidazolate Glasses through Topological Constraint Theory. *Journal of Physical Chemistry Letters*, **2018**, 9, 6985-6990 | 6.4 | 21 |
| 202 | Si/C/H ReaxFF Reactive Potential for Silicon Surfaces Grafted with Organic Molecules. *Journal of Physical Chemistry C*, **2018**, 122, 23515-23527 | 3.8 | 12 |
| 201 | ReaxFF Molecular Dynamics Study on the Influence of Temperature on Adsorption, Desorption, and Decomposition at the Acetic Acid/Water/ZnO(101 0) Interface Enabling Cold Sintering. *ACS Applied Materials & Interfaces*, **2018**, 10, 37717-37724 | 9.5 | 25 |
| 200 | Enabling Computational Design of ZIFs Using ReaxFF. *Journal of Physical Chemistry B*, **2018**, 122, 9616-9624 | 3.4 | 30 |
| 199 | ReaxFF simulations of petroleum coke sulfur removal mechanisms during pyrolysis and combustion. *Combustion and Flame*, **2018**, 198, 146-157 | 5.3 | 31 |
| 198 | Discovery of Descriptors for Stable Monolayer Oxide Coatings through Machine Learning. *ACS Applied Energy Materials*, **2018**, 1, 6217-6226 | 6.1 | 11 |
| 197 | Effect of chemical structure on thermo-mechanical properties of epoxy polymers: Comparison of accelerated ReaxFF simulations and experiments. *Polymer*, **2018**, 158, 354-363 | 3.9 | 27 |
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