Adri van Duin

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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	ReaxFF: A Reactive Force Field for Hydrocarbons. *Journal of Physical Chemistry A*, **2001**, 105, 9396-9409	2.8	3390
348	ReaxFF reactive force field for molecular dynamics simulations of hydrocarbon oxidation. *Journal of Physical Chemistry A*, **2008**, 112, 1040-53	2.8	1392
347	The ReaxFF reactive force-field: development, applications and future directions. *Npj Computational Materials*, **2016**, 2,	10.9	858
346	ReaxFFSiO Reactive Force Field for Silicon and Silicon Oxide Systems. *Journal of Physical Chemistry A*, **2003**, 107, 3803-3811	2.8	682
345	Shock waves in high-energy materials: the initial chemical events in nitramine RDX. *Physical Review Letters*, **2003**, 91, 098301	7.4	416
344	A reactive molecular dynamics simulation of the silica-water interface. *Journal of Chemical Physics*, **2010**, 132, 174704	3.9	359
343	Development of the ReaxFF reactive force field for describing transition metal catalyzed reactions, with application to the initial stages of the catalytic formation of carbon nanotubes. *Journal of Physical Chemistry A*, **2005**, 109, 493-9	2.8	332
342	Simulations on the thermal decomposition of a poly(dimethylsiloxane) polymer using the ReaxFF reactive force field. *Journal of the American Chemical Society*, **2005**, 127, 7192-202	16.4	316
341	Thermal decomposition of RDX from reactive molecular dynamics. *Journal of Chemical Physics*, **2005** , 122, 54502	3.9	313
340	Evaluation of B3LYP, X3LYP, and M06-Class Density Functionals for Predicting the Binding Energies of Neutral, Protonated, and Deprotonated Water Clusters. *Journal of Chemical Theory and Computation*, **2009**, 5, 1016-26	6.4	276
339	Development and Validation of ReaxFF Reactive Force Field for Hydrocarbon Chemistry Catalyzed by Nickel. *Journal of Physical Chemistry C*, **2010**, 114, 4939-4949	3.8	236
338	Combustion of an Illinois No. 6 coal char simulated using an atomistic char representation and the ReaxFF reactive force field. *Combustion and Flame*, **2012**, 159, 1272-1285	5.3	226
337	Multiparadigm modeling of dynamical crack propagation in silicon using a reactive force field. *Physical Review Letters*, **2006**, 96, 095505	7.4	194
336	Initiation mechanisms and kinetics of pyrolysis and combustion of JP-10 hydrocarbon jet fuel. *Journal of Physical Chemistry A*, **2009**, 113, 1740-6	2.8	184
335	Development of a ReaxFF potential for carbon condensed phases and its application to the thermal fragmentation of a large fullerene. *Journal of Physical Chemistry A*, **2015**, 119, 571-80	2.8	167
334	Effect of Metal Ion Intercalation on the Structure of MXene and Water Dynamics on its Internal Surfaces. *ACS Applied Materials & Interfaces*, **2016**, 8, 8859-63	9.5	164
333	Aqueous proton transfer across single-layer graphene. *Nature Communications*, **2015**, 6, 6539	17.4	159

332	Delft molecular mechanics: a new approach to hydrocarbon force fields. Inclusion of a geometry-dependent charge calculation. *Journal of the Chemical Society, Faraday Transactions*, **1994**, 90, 2881		156
331	Development of a ReaxFF reactive force field for glycine and application to solvent effect and tautomerization. *Journal of Physical Chemistry B*, **2011**, 115, 249-61	3.4	150
330	Catalyzed growth of carbon nanotube with definable chirality by hybrid molecular dynamics-force biased Monte Carlo simulations. *ACS Nano*, **2010**, 4, 6665-72	16.7	149
329	Reactive Potentials for Advanced Atomistic Simulations. *Annual Review of Materials Research*, **2013**, 43, 109-129	12.8	147
328	Development of a reactive force field for iron-oxyhydroxide systems. *Journal of Physical Chemistry A*, **2010**, 114, 6298-307	2.8	145
327	The utility of coal molecular models. *Fuel Processing Technology*, **2011**, 92, 718-728	7.2	143
326	Development and validation of a ReaxFF reactive force field for Cu cation/water interactions and copper metal/metal oxide/metal hydroxide condensed phases. *Journal of Physical Chemistry A*, **2010**, 114, 9507-14	2.8	140
325	Hydration of calcium oxide surface predicted by reactive force field molecular dynamics. *Langmuir*, **2012**, 28, 4187-97	4	139
324	Atomistic-scale simulations of the initial chemical events in the thermal initiation of triacetonetriperoxide. *Journal of the American Chemical Society*, **2005**, 127, 11053-62	16.4	136
323	Early maturation processes in coal. Part 2: Reactive dynamics simulations using the ReaxFF reactive force field on Morwell Brown coal structures. *Organic Geochemistry*, **2009**, 40, 1195-1209	3.1	134
322	A roadmap for electronic grade 2D materials. *2D Materials*, **2019**, 6, 022001	5.9	133
321	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
320	ReaxFF reactive force field development and applications for molecular dynamics simulations of ammonia borane dehydrogenation and combustion. *Journal of Physical Chemistry A*, **2010**, 114, 5485-92	2.8	124
319	Lithium ion solvation and diffusion in bulk organic electrolytes from first-principles and classical reactive molecular dynamics. *Journal of Physical Chemistry B*, **2015**, 119, 1535-45	3.4	123
318	Oxidation of Silicon Carbide by O2 and H2O: A ReaxFF Reactive Molecular Dynamics Study, Part I. *Journal of Physical Chemistry C*, **2012**, 116, 16111-16121	3.8	123
317	Water adsorption on stepped ZnO surfaces from MD simulation. *Surface Science*, **2010**, 604, 741-752	1.8	122
316	Reactions of singly-reduced ethylene carbonate in lithium battery electrolytes: a molecular dynamics simulation study using the ReaxFF. *Journal of Physical Chemistry A*, **2012**, 116, 2978-85	2.8	121
315	Dynamics of confined reactive water in smectite clay-zeolite composites. *Journal of the American Chemical Society*, **2012**, 134, 3042-53	16.4	113

314	A reactive force field (ReaxFF) for zinc oxide. *Surface Science*, **2008**, 602, 1020-1031	1.8	113
313	Extension of the ReaxFF Combustion Force Field toward Syngas Combustion and Initial Oxidation Kinetics. *Journal of Physical Chemistry A*, **2017**, 121, 1051-1068	2.8	110
312	Dynamics of the dissociation of hydrogen on stepped platinum surfaces using the ReaxFF reactive force field. *Journal of Physical Chemistry B*, **2006**, 110, 4274-82	3.4	110
311	ReaxFF molecular dynamics simulations on lithiated sulfur cathode materials. *Physical Chemistry Chemical Physics*, **2015**, 17, 3383-93	3.6	109
310	Formation of incipient soot particles from polycyclic aromatic hydrocarbons: A ReaxFF molecular dynamics study. *Carbon*, **2017**, 121, 380-388	10.4	107
309	Development and Application of a ReaxFF Reactive Force Field for Oxidative Dehydrogenation on Vanadium Oxide Catalysts. *Journal of Physical Chemistry C*, **2008**, 112, 14645-14654	3.8	106
308	Molecular dynamics simulations of stability of metal-organic frameworks against H2O using the ReaxFF reactive force field. *Chemical Communications*, **2010**, 46, 5713-5	5.8	105
307	Molecular dynamic simulation of aluminum□water reactions using the ReaxFF reactive force field. *International Journal of Hydrogen Energy*, **2011**, 36, 5828-5835	6.7	101
306	Atomistic-scale simulations of chemical reactions: Bridging from quantum chemistry to engineering. *Nuclear Instruments & Methods in Physics Research B*, **2011**, 269, 1549-1554	1.2	99
305	Plasma-Induced Destruction of Bacterial Cell Wall Components: A Reactive Molecular Dynamics Simulation. *Journal of Physical Chemistry C*, **2013**, 117, 5993-5998	3.8	95
304	ReaxFF Reactive Force-Field Study of Molybdenum Disulfide (MoS). *Journal of Physical Chemistry Letters*, **2017**, 8, 631-640	6.4	94
303	Atomistic-Scale Simulations of Defect Formation in Graphene under Noble Gas Ion Irradiation. *ACS Nano*, **2016**, 10, 8376-84	16.7	92
302	Pyrolysis of a large-scale molecular model for Illinois no. 6 coal using the ReaxFF reactive force field. *Journal of Analytical and Applied Pyrolysis*, **2014**, 109, 79-89	6	92
301	Molecular Dynamics Simulations of the Oxidation of Aluminum Nanoparticles using the ReaxFF Reactive Force Field. *Journal of Physical Chemistry C*, **2015**, 119, 17876-17886	3.8	91
300	Mechanical properties of amorphous LixSi alloys: a reactive force field study. *Modelling and Simulation in Materials Science and Engineering*, **2013**, 21, 074002	2	91
299	ReaxFF Reactive Force Field Study of the Dissociation of Water on Titania Surfaces. *Journal of Physical Chemistry C*, **2013**, 117, 10558-10572	3.8	91
298	In situ atomistic insight into the growth mechanisms of single layer 2D transition metal carbides. *Nature Communications*, **2018**, 9, 2266	17.4	89
297	Development of the ReaxFF reactive force field for mechanistic studies of catalytic selective oxidation processes on BiMoO x. *Topics in Catalysis*, **2006**, 38, 93	2.3	89

296	Molecular dynamics simulations of laser-induced incandescence of soot using an extended ReaxFF reactive force field. *Journal of Physical Chemistry A*, **2010**, 114, 12561-72	2.8	87
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294	Physical mechanism of anisotropic sensitivity in pentaerythritol tetranitrate from compressive-shear reaction dynamics simulations. *Applied Physics Letters*, **2010**, 96, 081918	3.4	83
293	Thermal decomposition process in algaenan of Botryococcus braunii race L. Part 2: Molecular dynamics simulations using the ReaxFF reactive force field. *Organic Geochemistry*, **2009**, 40, 416-427	3.1	82
292	A divide-and-conquer/cellular-decomposition framework for million-to-billion atom simulations of chemical reactions. *Computational Materials Science*, **2007**, 38, 642-652	3.2	82
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288	Development of a ReaxFF reactive force field for titanium dioxide/water systems. *Langmuir*, **2013**, 29, 7838-46	4	77
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285	Thermal properties of fluorinated graphene. *Physical Review B*, **2013**, 87,	3.3	75
284	Comparison of thermal and catalytic cracking of 1-heptene from ReaxFF reactive molecular dynamics simulations. *Combustion and Flame*, **2013**, 160, 766-775	5.3	73
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277	Molecular dynamics simulations of the effects of vacancies on nickel self-diffusion, oxygen diffusion and oxidation initiation in nickel, using the ReaxFF reactive force field. *Acta Materialia*, **2015**, 83, 102-112	8.4	65
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269	eReaxFF: A Pseudoclassical Treatment of Explicit Electrons within Reactive Force Field Simulations. *Journal of Chemical Theory and Computation*, **2016**, 12, 3463-72	6.4	59
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263	Oxidation-assisted ductility of aluminium nanowires. *Nature Communications*, **2014**, 5, 3959	17.4	55
262	The ReaxFF Monte Carlo reactive dynamics method for predicting atomistic structures of disordered ceramics: application to the Mo(3)VO(x) catalyst. *Angewandte Chemie - International Edition*, **2009**, 48, 7630-4	16.4	55
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253	Structures, Energetics, and Reaction Barriers for CHx Bound to the Nickel (111) Surface. *Journal of Physical Chemistry C*, **2009**, 113, 20290-20306	3.8	51
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248	Role of Site Stability in Methane Activation on PdxCe1−xO2−δ Surfaces. *ACS Catalysis*, **2015**, 5, 6187-6199	13.1	47
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245	Tribochemistry of Phosphoric Acid Sheared between Quartz Surfaces: A Reactive Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2013**, 117, 25604-25614	3.8	46
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241	Tunable nanomechanics of protein disulfide bonds in redox microenvironments. *Journal of the Mechanical Behavior of Biomedical Materials*, **2012**, 5, 32-40	4.1	45
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236	Pyrolysis of binary fuel mixtures at supercritical conditions: A ReaxFF molecular dynamics study. *Fuel*, **2019**, 235, 194-207	7.1	42
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233	ReaxFF molecular dynamics simulation of thermal stability of a Cu3(BTC)2 metal-organic framework. *Physical Chemistry Chemical Physics*, **2012**, 14, 11327-32	3.6	41
232	Graphene reinforced carbon fibers. *Science Advances*, **2020**, 6, eaaz4191	14.3	40
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225	Modeling of molecular nitrogen collisions and dissociation processes for direct simulation Monte Carlo. *Journal of Chemical Physics*, **2014**, 141, 234307	3.9	37

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221	Characterization of the active site of yeast RNA polymerase II by DFT and ReaxFF calculations. *Theoretical Chemistry Accounts*, **2008**, 120, 479-489	1.9	36
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214	Phase transitions of ordered ice in graphene nanocapillaries and carbon nanotubes. *Scientific Reports*, **2018**, 8, 3851	4.9	33
213	Reactive adsorption of ammonia and ammonia/water on CuBTC metal-organic framework: a ReaxFF molecular dynamics simulation. *Journal of Chemical Physics*, **2013**, 138, 034102	3.9	33
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