**Curriculum Vitae**

**ADRI C.T. VAN DUIN**

## **Distinguished University Professor**

## **Professor, Mechanical Engineering**

**Professor, Chemical Engineering (courtesy)**

**Professor, Engineering Science and Mechanics (courtesy)**

**Professor, Chemistry (courtesy)**

**Professor, Materials Science and Engineering (courtesy)**

**Director of the Materials Computation Center**

**CTO, RxFF\_Consulting.LLC**

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**Education and Training:**

University of Amsterdam, the Netherlands Chemistry Drs. 1991

Delft University of Technology the Netherlands Chemistry PhD 1996

# Professional experience

2021-current Distinguished University Professor

2015-current Professor at the Department of Mechanical Engineering, Penn State

2015-current Director of the Materials Computation Center, Penn State

2013-current CTO and co-founder, RxFF\_Consulting.LLC

2008-2015 Associate Professor at the Department of Mechanical Engineering, Pennsylvania State University, University Park, PA.

2003-2008 Postdoctoral researcher (2003-2005), research faculty (2005-2007) and Senior research staff (2007-2008), California Institute of Technology, Pasadena, CA

1996-2002 Postdoctoral Researcher at the University of Newcastle upon Tyne, United Kingdom.

**Awards and Honors**

- 1997 Marie Curie Fellowship (1997-1999)

- 1999 Royal Society University Research Fellowship (1999-2002)

- 2012 Penn State Engineering Alumni Society Outstanding Research Award

- 2015 Awarded the Kenneth Kuan-Yun Kuo Early Career Professorship (Jan 2015-Dec 2017)

- 2017 Awarded the Penn State Faculty Scholar Medal

- 2017 Award from the Japanese Association for Chemical Innovation

- 2020 Elected as Full Member of Sigma XI

- 2021 Awarded title of Distinguished University Professor

**Research Interests and impact**: Adri van Duin is the inventor and main developer of the ReaxFF reactive force field method, which enables fully dynamical, fully reactive atomistic-scale simulations for complex materials, molecules and their interfaces. Applications include combustion, catalysis, energy storage, biomaterials and material failure.

The ReaxFF method is currently used by over 2000 academic and industrial groups around the world. The ReaxFF method is incorporated in various major computational materials software packages, like LAMMPS (released by Sandia National Labs) and ADF (released by SCM Amsterdam). Since 2015 the ReaxFF force fields and examples have been distributed through requests at the Material Computation Center website at Penn State – this has resulted, so far, in over 25,000 requests demonstrating the global impact of this method.

The global impact of this work is also reflected in publication co-author distributions – showing collaborators from a wide range of countries, see the Penn State PURE site (<https://pennstate.pure.elsevier.com/en/persons/adri-van-duin>)

**Teaching contributions.** Dr. van Duin has been teaching undergraduate thermodynamics courses at the 300 and the 400 level – specifically the ME-300 and ME-400 courses. At the graduate level he has been teaching courses about spectroscopy and statistical thermodynamics (ME-535, Physics of Gases), has co-taught a graduate course on combustion chemistry (ME-532). Furthermore, he has developed a new course, ME/ChE 505, named ‘Atomistic-scale simulations for engineers’, which is cross-listed between Mechanical Engineering and Chemical Engineering. This course has been offered six times so far and seeks to introduce engineering students to atomistic-scale simulation methods, in particular Density Functional Theory, reactive and non-reactive force fields. The course has attracted students from various departments and colleges, including material scientists, chemists and mechanical/chemical/electrical and nuclear engineers. The course includes a final project – and four of these projects have culminated into peer-reviewed journal publications.

**Service contributions**. Below is a summary of Dr. van Duin’s Penn State service contributions for the last six years.

**2023**

* Director of the Material Computation Center, one of the four centers within the Material Research Institute (MRI)
* Chair of the Faculty Scholar Medal committee in Engineering
* Organizer, Mechanical Engineering Faculty Retreat – Research Super Group session
* Reviewer for the Institute of Computational and Data Science seed grant proposals
* Faculty mentor for two mechanical engineering assistant professors
* Chair of the Mechanical Engineering Research Advancement committee
* Member of the ME-300 (Thermodynamics) course caucus

**2022**

* Director of the Material Computation Center, one of the four centers within the Material Research Institute (MRI)
* Chair of the Faculty Scholar Medal committee in Engineering
* Organizer, Mechanical Engineering Faculty Retreat – Research Super Group session
* Member of the Institute for Computation and Data Science (ICDS) Coordinating Committee
* Reviewer for the Institute of Computational and Data Science seed grant proposals
* Faculty mentor for two mechanical engineering assistant professors
* Member of the Mechanical Engineering Research Advancement committee
* Member of the ME-300 (Thermodynamics) course caucus

**2021**

* Director of the Material Computation Center, one of the four centers within the Material Research Institute (MRI)
* Member of a AC14 Review committee for evaluating a department in the College of Engineering
* Organizer, Mechanical Engineering Faculty Retreat – Faculty Lightning-presentation session.
* Member of the Institute for Computation and Data Science (ICDS) Coordinating Committee
* Faculty mentor for two mechanical engineering assistant professors
* Member of the Mechanical Engineering Teaching Load Policy Committee
* Member of the ME-300 (Thermodynamics) course caucus

**2020**

* Director of the Material Computation Center, one of the four centers within the Material Research Institute (MRI)
* Member of the Institute for Computation and Data Science (ICDS) Coordinating Committee
* Co-chair of the Research Computing and CyberInfrastructure (RCCI) Advisory Council
* Member of the RCCI working group for High-Performance Computing
* Member of the Mechanical Engineering Teaching Load Policy Committee
* Member of the Mechanical Engineering Research Advancement Committee
* Member of the ME-300 (Thermodynamics) course caucus
* Faculty mentor for two mechanical engineering assistant professors

**2019**

* Director of the Material Computation Center, one of the four centers within the Material Research Institute (MRI)
* Member of the Institute for Computation and Data Science (ICDS) Coordinating Committee
* Co-chair of the Research Computing and CyberInfrastructure (RCCI) Advisory Council
* Chair of the RCCI Working group for High-Performance Computing
* Member of the Mechanical Engineering Research Advancement Committee
* Member of the ME-300 (Thermodynamics) course caucus
* Faculty mentor for one mechanical engineering assistant professor

**2018**

* Director of the Material Computation Center, one of the four centers within the Material Research Institute (MRI)
* Member of the Institute for Computation and Data Science (ICDS) Coordinating Committee
* Chair of the RCCI Working group for High-Performance Computing
* Chair of the College of Engineering Computing Working Group
* Member of the Mechanical Engineering Faculty Search Committee for Emerging Areas
* Member of the Mechanical Engineering Promotion/Tenure committee
* Member of the Mechanical Engineering Research Advancement Committee
* Member of the ME-300 (Thermodynamics) course caucus

External services contributions include:

* Associate Editorship for the *Carbon* journal (2021-2022) (2020 Impact Factor 9.594)
* Reviewing for a wide range of chemistry, Physical Chemistry and Materials journals, including Nature Materials, Nature Computational Materials, Nature Communications, Journal of the American Chemical Society, Carbon, Energy&Fuels, Journal of Physical Chemistry, Physical Reviews Letters.
* Associate Editor of the International Journal for Energetic Materials and Chemical Propulsion from 2009-2014.
* Reviewed proposals for NSF, DoE, various DoD agencies and a number of funding agencies abroad, in particular the Danish Council for Research (Denmark), the Flemish Council for research (NSF Belgium), the Deutsche Forchungsgemeinschaft (DFG, Germany), the Royal Society (United Kingdom), the Israel Science Foundation (ISF) and the US/Israel Binational Science Foundation (BSF).
* Serves as the external advisor for a Jet Propulsion Laboratory (JPL) project related to the atmospheric chemistry of Enceladus (one of Saturn’s moons).

# Journal publications.

# Citations: 43900; h-index: 101 (source: Google Scholar, September 2023)

1. Zhu, H., Nayir, N., Choudhury, T.H., Bansal, A., Huet, B., Kunyan, Z., Puretzky, A., Bachu, S., Krystal, Y., McKnight, T.V., Trainor, N., Durbin, S., Huang, S., Alem, N., van Duin, A.C.T., Crespi, V.H. and Redwing, J. (2023) Step engineering for nucleation and domain orientation control in WSe2 epitaxy on c-plane sapphire. Nature Nanotechnology **https://doi.org/10.1038/s41565-023-01456-6.**
2. Zhang, L., Kowalik, M., Mao, Q., Damirchi, B., Zhang, Y., Bradford, P.D., Li, Q., van Duin, A.C.T. and Zhu, Y.T. (2023) Joint theoretical and experimental study of stress graphitization in aligned carbon nanotube/carbon matrix composite. ACS Applied Materials & Interfaces **15**, 32656-32666.
3. Yousefian, P., Sepehrinezhad, A., van Duin, A.C.T. and Randall, C. (2023) Improved Prediction for Failure Time of Multilayer Ceramic Capacitors (MLCCs): A Physics-based Machine Learning Approach. APL Machine Learning **1**.
4. Yang, Y., Shin, Y.K., Murase, Y., Kawata, S., Keino, D., Kolbe, J., Berbano, S., Zhang, X., van Duin, A.C.T. and Mauro, J.C. (2023) Aqueous stability of MOFs using ReaxFF-based Metadynamics Simulation. Journal of Physical Chemistry B **published online**.
5. Tsai, W.-Y., Boyd, S., Ganeshan, K., Saeed, S., Gao, Y., van Duin, A.C.T., Augustyn, V. and Balke, N. (2023) Effect of electrode/electrolyte coupling on birnessite (-MnO2) mechanical response and degradation. ACS Applied Materials & Interfaces **published online.**
6. Schulze, J.A., Yilmaz, D., Cable, M., Malaska, M., Hofman, A., Hodyss, R., Lunine, J., van Duin, A. and Jaramillo-Botero, A. (2023) The effect of salts in the formation and hypervelocity-induced fragmentation of icy clusters with embedded amino acids. ACS Earth and Space Chemistry **7**, 168-181.
7. Park, H., van Duin, A.C.T. and Koposov, A. (2023) Toward Atomistic Understanding of Materials with Conversion-Alloying Mechanism in Li-ion Batteries. Chemistry of Materials **35**, 2835-2845.
8. Oviroh, P., Jen, T.-C., Ren, J. and van Duin, A.C.T. (2023) Towards the Realisation of High Permi-Selective MoS2 Membrane for Water Desalination. npj Clean Water **14**.
9. Nayir, N., Mao, Q., Wang, T., Kowalik, M., Zhang, Y., Wang, M., Dwivedi, S., Jeong, G.-U., Shin, Y.K. and van Duin, A.C.T. (2023) Modeling and Simulations for 2D Materials: A ReaxFF perspective. 2D Materials **10**, 032002.
10. Nayir, N., Bartolucci, S.F., Wang, T., Chen, C., Maurer, J.A., Redwing, J. and van Duin, A.C.T. (2023) Modulation effect of Substrate Interactions on Nucleation and Growth of MoS2 on Silica. Journal of Physical Chemistry C **127**, 9039-9048.
11. Mohammadtabar, K., Guerrero, E., Romero Garcia, S., Shin, Y.K., van Duin, A.C.T., Strubbe, D. and Martini, A. (2023) Development and Demonstration of a ReaxFF Reactive Force Field for Ni-Doped MoS2. Journal of Physical Chemistry C **published online**.
12. Mao, Q., Feng, M., Jiang, X.Z., Ren, Y., Luo, K. and van Duin, A.C.T. (2023) Classical and Reactive Molecular Dynamics: Principles and Applications in Combustion and Energy Systems. Progress in Energy and Combustion Science **97**, 101084.
13. Lin, Y.-C., Torsi, R., Nayir, N., Rajabpour, S., van Duin, A.C.T., Law, S., Jaramillo, R., Engel-Herbert, R., Wang, Y., Terrones, M., Redwing, J., Terrones, M. and Robinson, J. (2023) Recent Advances in 2D Material Theory, Synthesis, Properties, and Applications. ACS Nano **published online**.
14. Krstic, P., Ostrowski, E.T., Maan, A., Abe, S., Dwivedi, S., van Duin, A.C.T. and Koel, B.E. (2023) Processes at lithium-hydride/deuteride surfaces upon low energy impact of H/D. Frontiers of Physics **published online**.
15. Krstic, P., Ostrowski, E.T., Abe, S., Maan, A., Dwivedi, S., van Duin, A.C.T. and Koel, B.E. (2023) Detailed Studies of the Processes in Low Energy H Irradiation of Li and Li-Compound Surfaces. Journal of Applied Physics **published online.**
16. Kritikos, E., Lele, A., van Duin, A.C.T. and Giusti, A. (2023) Atomistic insight into the effects of electrostatic fields on hydrocarbon reaction kinetics Journal of Chemical Physics **published online.**
17. Guifo, S.B.O.o., Mueller, J.E., van Duin, D., Talkhoncheh, M.K., van Duin, A.C.T., Henriques, D. and Markus, T. (2023) Development and validation of a ReaxFF reactive force field describing silicon/carbon composite anode materials for lithium-ion batteries. Journal of Physical Chemistry C **127**, 2818-2834.
18. Gallegos, I., Kemppainen, J., Gissinger, J.R., Kowalik, M., van Duin, A.C.T., Wise, K.E., Gowtham, S. and Odegard, G.M. (2023) Establishing Physical and Chemical Mechanisms of Polymerization and Pyrolysis of Phenolic Resins for Carbon-Carbon Composites. Carbon Trends **12**, 100290.
19. Gaikwad, P., Mondal, K., Shin, Y.K., van Duin, A.C.T. and Pawar, G. (2023) Enhancing the Faradaic Efficiency of Solid Oxide Electrolysis Cells: Progress and Perspective npj Computational Materials **9**, 149.
20. Fortunato, J., Shin, Y.K., Spencer, M.A., van Duin, A.C.T. and Augustyn, V. (2023) Choice of Electrolyte Impacts the Selectivity of Electrochemical PCET Reactions on Hydrogen Titanate Journal of Physical Chemistry C **accepted for publication**.
21. Dhakane, A., Xie, T., Yilmaz, D., van Duin, A.C.T., Sumpter, B.G. and Ganesh, P. (2023) A Graph Dynamical Neural Network Approach for Decoding Dynamical States in Ferroelectrics. Carbon Trends **11**, 100264.
22. Chin, J., Frye, M., Liu, D.S.-H., Hilse, M., Graham, I., Shallenberger, J., Wang, K., Engel-Herbert, R., Wang, M., Shin, Y.K., Nayir, N., van Duin, A.C.T. and M., G.L. (2023) Self-Limiting Stoichiometry in SnSe Thin Films Nanoscale **15**, 9973.
23. Bachu, S., Kowalik, M., Huet, B., Nayir, N., Dwivedi, S., Hickey, D.R., Qian, C., Snyder, D.W., Redwing, J., van Duin, A.C.T. and Alem, N. (2023) Role of Bilayer Graphene Microstructure on the Nucleation of WSe2 Overlayers. ACS Nano **17**, 12140-12160.
24. Ahmad, W., Koley, P., Dwivedi, S., Lakshman, R., Shin, Y.K., van Duin, A.C.T., Shrotri, A. and Tanksale, A. (2023) Aqueous phase conversion of CO2 into acetic acid over thermally transformed MIL-88B. Nature Communications **14**, 2821-2821.
25. Zhu, W., Boyer, E., Yetter, R.A. and van Duin, A.C.T. (2022) A Kinetic Study of Solid Carbon Fuel Conversions in Cu-based Chemical Looping Combustion Process Using the ReaxFF Reactive Force Field Approach. Combustion and Flame **244**, 112216.
26. Xu, Q., Zhang, J., Li, X., van Duin, D.M., Hu, Y., van Duin, A.C.T. and Ma, T. (2022) How polytetrafluoroethylene lubricates iron: an atomistic view by Reactive Molecular Dynamics. ACS Applied Materials & Interfaces **14**, 6239-6250.
27. Sengul, M.Y., Ndayishimiye, A., Lee, W., Seo, J.-H., Fan, Z., Shin, Y.K., Gomez, E.D., Randall, C.A. and van Duin, A.C.T. (2022) Understanding the aqueous dissolution dynamics of NASICON-type Li1+xAlxTi2-x(PO4)3 (LATP) a. Phys. Chem. Chem. Phys. **24**, 4125.
28. Schulze, J.A., Kowalik, M., Hua, M., We, S., Alsaid, Y., He, X. and van Duin, A.C.T. (2022) Investigation of Mechanical Properties in PVA Hydrogels Due to Cation Interactions Described by Reactive Forcefield Based Molecular Dynamics Simulations. Journal of the Minerals, Metals and Materials Society **74**, 4632-4639.
29. Sakib, N., Paul, S., Akash, T.S., Nayir, N., van Duin, A.C.T. and Momeni, K. (2022) Role of tilt grain boundaries on the structural integrity of WSe2 monolayers. Phys. Chem. Chem. Phys. **18**, 27241-27249.
30. Prenger, K., Sun, Y., Ganeshan, K., Al-Temimy, A., Liang, K., Xiao, J., Pettit, T., van Duin, A.C.T., Jiang, D.-e. and Naguib, M. (2022) Metal Cation Pre-Intercalated Ti3C2Tz MXene as High Areal Capacitance Electrodes for Aqueous Supercapacitors. ACS Applied Energy Materials, **5**, 9373-9382.
31. Pols, M., Hilpert, T., Filot, I., van Duin, A.C.T., Calero, S. and Tao, S. (2022) What Happens at Surfaces and Grain Boundaries of Halide Perovskites: Insights from Reactive Molecular Dynamics Simulations of CsPbI3. ACS Applied Materials & Interfaces **14**, 40841-40850.
32. Onwudinanti, C., Pols, M., Brocks, G., Koelman, V., van Duin, A.C.T., Morgan, T. and Tao, S. (2022) A molecular dynamics study of hydrogen diffusion in ruthenium. Journal of Physical Chemistry **126**, 5950-5959.
33. Nayir, N., Sengul, M.Y., Costine, A.L., Reinke, P., Rajabpour, S., Bansal, A., Kozhakhmetov, A., Robinson, J., Redwing, J. and van Duin, A.C.T. (2022) Atomic-scale Probing of Defect-assisted Ga intercalation through Graphene using ReaxFF Molecular Dynamics Simulations. Carbon **190**, 276-290.
34. Momeni, K., Ji, Y., Nayir, N., Choudhury, T.H., Zhu, H., van Duin, A.C.T., Redwing, J. and Chen, L.-Q. (2022) A Computational Framework for Guiding the MOCVD-Growth of Wafer-Scale 2D Materials. npj Computational Materials **240**, 108.
35. Mao, Q., Zhang, Y., Kowalik, M., Nayir, N., Chandross, M. and van Duin, A.C.T. (2022) Oxidation and Hydrogenation of Monolayer MoS2 with Compositing Agent under Environmental Exposure: The ReaxFF Mo/Ti/Au/O/S/H Force Field Development and Applications. Frontier in Nanoscience **4**, 1034795.
36. Mao, Q., Rajabpour, S., Talkhoncheh, M.K., Zhu, J., Kowalik, M. and van Duin, A.C.T. (2022) Cost-Effective Carbon Fiber Precursor Selections of Polyacrylonitrile-Based Blend Polymers: Carbonization Chemistry and Structural Characterizations. Nanoscale **4**, 6357.
37. Leyssale, J.-M., Valdenaire, P.-L., Pellenq, R., van Duin, A.C.T. and Galvez, M. (2022) Atomic-scale mechanism of carbon nucleation from a deep crustal fluid by replica exchange reactive molecular dynamics simulation. Geochim. Cosmochim. Acta **329**, 106-118.
38. Lele, A., Krstic, P. and van Duin, A.C.T. (2022) ReaxFF force field training for gas phase hBN nanostructure synthesis. Journal of Physical Chemistry A **126**, 568-582.
39. Kritikos, E., Lele, A., van Duin, A.C.T. and Giusti, A. (2022) Electric Field Effects on n-Dodecane Combustion: a Reactive Molecular Dynamics Study. Combustion and Flame **244**, 112238.
40. Kelley, K.P., Morozovska, A.N., Eliseev, E.A., Sharma, V., Yilmaz, D., van Duin, A.C.T., Panchapakesan, G., Borisevich, A., Jesse, S., Maksymovych, P., Balke, N., Kalinin, S.V. and Vasudevan, R.K. (2022) Oxygen vacancy injection as a pathway to enhancing electromechanical response in ferroelectrics. Advanced Materials **34**, 2106426.
41. Kaymak, M.C., Rahnamoun, A., O’Hearn, K.A., van Duin, A.C.T., Merz, K.M.J. and Aktulga, H.M. (2022) JAX-ReaxFF: A Gradient Based Framework for Extremely Fast Optimization of Reactive Force Fields. Journal of Optimization Theory and Applications **18**, 5181-5194.
42. Kanski, M., Maciazek, D., Postawa, Z., van Duin, A.C.T. and Garrison, B.J. (2022) Development of a Charge-implicit ReaxFF description for C/H/O Systems. Journal of Physical Chemistry Letters **13**, 628-633.
43. Jacobson, A.T., Chen, C., Dewey, J.C., Copeland, G.C., Allen, W., Richards, B., Kaszuba, J.P., van Duin, A.C.T., Cho, H., Deo, M., She, Y. and Martin, T.P. (2022) Nanoscale pore geometries and the point of zero charge of synthesized silica materials. Journal of Colloid and Interface Science **8**, 100069.
44. Hou, D., Feng, M., Wei, J., Wang, Y., van Duin, A.C.T. and Luo, K. (2022) A reactive force  eld molecular dynamics study on the inception mechanism of titanium tetraisopropoxide (TTIP) conversion to titanium clusters. Chemical Engineering Journal **252**, 117496.
45. Hossain, M.J., Pawar, G. and van Duin, A.C.T. (2022) Development and applications of an eReaxFF force field for graphitic systems. Journal of the Electrochemical Society **169**, 110540.
46. Gupta, A., Khodayari, A., van Duin, A.C.T. and Seveno, D. (2022) Cellulose Nanocrystals: Tensile Strength and Failure mechanisms Revealed using Reactive Molecular Dynamics. Biomacromolecules **23**, 2243-2254.
47. Gao, Y., Zhu, W., Wang, T., Yilmaz, D.E. and van Duin, A.C.T. (2022) A C/H/O/F/Al ReaxFF Force Field Development and Application to Study the Condensed Phase Poly(vinylidene)-fluoride and Reaction Mechanisms with Aluminum. Journal of Physical Chemistry C **126**, 11058-11074.
48. Gao, Y., Pastrana, A.P.C., Manogharan, G. and van Duin, A.C.T. (2022) A Reactive Molecular Dynamics Study of Bi-modal Particle Size Distribution in Binder-Jetting Additive Manufacturing. Phys. Chem. Chem. Phys. **24**, 11603-11615.
49. Ganeshan, K., Khanal, R., Muraleedharan, M.G., Hellstrom, M., Kent, P.R.C., Irle, S. and van Duin, A.C.T. (2022) Importance of Nuclear Quantum Effects for Transport Under Confinement in Ti3C2 MXenes. Journal of Chemical Theory and Computation **18**, 6920-6931.
50. Gaikwad, P., Kowalik, M., van Duin, A.C.T. and Odegard, G.M. (2022) Computational study of Effect of Radiation Induced Crosslinking on the Properties of Flattened Carbon Nanotubes RSC Advances **12**, 28945.
51. Gaikwad, P., Kowalik, M., Jensen, B.D., van Duin, A.C.T. and Odegard, G.M. (2022) Improving Interfacial Interaction Between Flattened Carbon Nanotubes and Amorphous Carbon using Molecular Simulation. ACS Applied Nano Materials **5**, 5915-5924.
52. Fiesinger, F., Gaissmaier, D., van den Borg, M., Bessner, J., van Duin, A.C.T. and Jacob, T. (2022) Development of a Mg/O ReaxFF Potential to describe the Passivation Processes in Magnesium-Ion Batteries. ChemSusChem **16**, e202201821.
53. Farias, J.C., Paupitz, R., van Duin, A.C.T. and Bernal, M. (2022) Evaluation of the REAX force-field for studying the collision of an energetic proton with the DNA. Journal of Chemical Theory and Computation **18**, 6463-6471.
54. Dupuis, R., Hahn, S.H., van Duin, A.C.T. and Poulesquen, A. (2022) Condensation and Growth of Amorphous Aluminosilicate Nanoparticles by Aggregation Process. Journal of Physical Chemistry Letters 24, 9229.
55. Duong, P.H.H., Shin, Y.K., Kuehl, V.A., Afroz, M.M., Hoberg, J.O., Parkinson, B.A., van Duin, A.C.T. and Li-Oakey, K.D. (2022) Mechanistic Study of pH effect on organic solvent nanofiltration using carboxylated covalent organic framework as a modeling and experimental platform. Journal of Separation and Purification **282**.
56. Dasgupta, N., Chen, C. and van Duin, A.C.T. (2022) Development and Application of ReaxFF Methodology for Understanding the Chemical Dynamics of Metal Carbonates in Aqueous Solutions. Physical Chemistry Chemical Physics **24**, 3322-3337.
57. Clares, A.P., Gao, Y., Stebbins, R., Manogharan, G. and van Duin, A.C.T. (2022) Increasing Density and Mechanical Performance of Binder Jetting Processing via Bimodal Particle Size Distribution Materials Science in Additive Manufacturing **1**, 20.
58. Chazot, C.A.C., Damirchi, B., van Duin, A.C.T. and Hart, J. (2022) Meta-aramid/carbon nanotubes interaction in structural nanocomposites formed by in situ interfacial polymerization. Nano Letters **22**, 998-1006.
59. Campbell, I.E., Nayir, N., van Duin, A.C.T. and Mohney, S. (2022) N-Doping and Oxidation Dependence of Graphene Surface Reactivity During Vapor Deposition of Platinum Journal of Physical Chemistry **126**, 16357-16368.
60. Bansal, A., Nayir, N., Wang, K., Rondomanski, P., Subramanian, S., Kumari, S., Robinson, J.A., van Duin, A.C.T. and Redwing, J.M. (2022) Towards a mechanistic understanding of the formation of 2D-GaNx in epitaxial graphene. ACS Nano **17**, 230-239.
61. Bang, S.H., Sengul, M.Y., Fan, Z., Ndayishimiye, A., van Duin, A.C.T. and Randall, C.A. (2022) Morphological and chemical evolution of transient interfaces during zinc oxide cold sintering process. Materials Today Chemistry **24**, 100925.
62. Banerjee, R., Granzier-Nakajima, T., Lele, A., Schulze, J.A., Hossain, M.J., Zhu, W., Pabbi, L., Kowalik, M., van Duin, A.C.T., Terrones, M. and Hudson, E.W. (2022) On the origin of non-classical ripples in draped graphene sheets. ACS Applied Nano Materials **5**, 10829-10838.
63. Afroz, M.M., Shin, Y.K., van Duin, A.C.T. and Li-Oakey, K.D. (2022) Reactive Force Field (ReaxFF) Simulation of Rigid Segment of Shape-memory Polyurethane to Enable on-demand Material Design and Synthesis. Journal of Applied Polymer Science **e54486**.
64. Yilmaz D., Woodward W. H. H. and van Duin A. C. T. (2021) Machine Learning Assisted Hybrid Reax Simulations *Journal of Chemical Theory and Computation* **17**, 6705-6712.
65. Verma A., Zhang W. and van Duin A. C. T. (2021) ReaxFF reactive molecular dynamics simulations to study the interfacial dynamics between defective h-BN nanosheet and water nanodroplets. *Physical Chemistry Chemical Physics* **23**, 10822-10834.
66. Urquiza M. L., Islam M., van Duin A. C. T., Cartoixa X. and Strachan A. (2021) Atomistic insights on the full operation cycle ofa HfO2-based RRAM cell from molecular dynamics. *ACS Nano* **15**,12945-12954.
67. Tsuji K., Sengul M. Y., Fan Z., Akbarian D., Bang S. H., Ndayishimiye A., van Duin A. C. T. and Randall C. A. (2021) Fundamental consideration of a novel chemically-driven low temperature densification route of inorganic materials in a molten oxosalts cold sintering. . *TBA*.
68. Shin Y. K., Gao Y., Shin D. and van Duin A. C. T. (2021) Impact of three-body interactions in a ReaxFF force field for Cr and Ni transition metals and their alloys on the prediction of thermal and mechanical properties *Computational Materials Science* **197**, 110602.
69. Shin Y. K., Ashraf C. and van Duin A. C. T. (2021) Development and applications of the ReaxFF reactive force field for biological systems. In *Computational Materials, Chemistry, and Biochemistry: From Bold Initiatives to the Last Mile (In Honor of William A. Goddard’s Contributions to Science and Engineering)* (ed. W. A. Goddard III). Springer International Publishing.
70. Sengul M. Y., Song Y., Nayir N., Gao Y., Hung Y., Dasgupta T. and van Duin A. C. T. (2021) An initial design-enhanced Deep Learning-based optimization framework to parameterize multicomponent ReaxFF force fields *Nature Computational Materials* **68**, 1-8.
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# Selected Conference activities- invited presentations

# van Duin, A.C.T., MRS meeting, in person, ‘Atomistic-scale simulations of realistic, complex, reactive materials: the ReaxFF method, its applications and recent developments’, 100-150 in attendance, invited (April 2023)

# van Duin, A.C.T., MARM meeting, in person ‘Atomistic-scale simulations of realistic, complex, reactive materials: the ReaxFF reactive force field and its academic and industrial application’, 50-100 in attendance, invited (June 2022)

# van Duin, A. C., Lorentz workshop, University of Leiden, the Netherlands, Online, "Background of the ReaxFF reactive force field and its applications to the simulation of exothermic reactions at surfaces," 60 in attendance, Invited. (May 17, 2022). International.

# van Duin, A. C., Graphene and beyond, State College, "Atomistic-scale simulations of realistic, complex, reactive materials: overview of the ReaxFF reactive force field and its applications to 2D materials," 100 in attendance, peer-reviewed/refereed, Invited. (May 1, 2022 - May 3, 2022). International.

# van Duin, A. C., Surface Science Forum, ASML, Online, "Atomistic-scale simulations of realistic, complex, reactive oxide/water interfaces: the ReaxFF reactive force field and its applications," 50 in attendance, Invited. (February 23, 2022). International.

# van Duin, A.C.T., Autochemo conference, online ‘The ReaxFF force field- application overview and new directions in accelerated dynamics, ferroelectric/2D materials and treatment of explicit electrons’, 150 in attendance, invited (December 2021)

# Professional Membership

# American Chemical Society

# American Physical Society

# Material Research Society

# American Institute for Chemical Engineering

# Sigma XI

**Graduate advisors**: Prof. J.W. de Leeuw, prof. H. van Bekkum and Dr. B. van de Graaf (Delft University of Technology, the Netherlands)

**Postdoctoral advisors**: Prof. S.R. Larter (University of Newcastle upon Tyne, UK, currently U. Calgary) and Prof. W.A. Goddard (California Institute of Technology)

**Current and past students and postdocs**:

*Past students and postdocs:* Satyam Agrawalla (MSc, graduated summer 2010, currently MicroStrategy), Arvind Bharati (MSc, graduated Fall 2011, currently Steer Engineering), Shashank Singhai (MSc, graduated Fall 2011, currently John Deere), Amar Kamat (MSc, graduated Spring 2011, currently postdoc U.Groningen), Kauhik Joshi (PhD, Summer 2012, currently U.Virginia), Dr. Mike Russo (Electric Grid, Philadelphia), Sung-Yup Kim (PhD, Fall 2012, currently KIST), Osvalds Verners (PhD, summer 2014, currently Delft University of Technology) Mahdi Golkaram (MSc, Spring 2014, currently PhD at USB), Dr. Nitin Kumar (currently U.Boulder), Dr. Michael Weismiller (currently DoE), Chenyu Zou (PhD Fall 2014, currently CGGveritas), Murali Raju (PhD Fall 2014, currently Stanford U.), Sriram Srinivasan (PhD Fall 2014, currently Tata Industries), Dr. George Psofogiannakis (currently U.Ottawa), Thomas Senftle (PhD Summer 2015, currently Rice U.), Jejoon Yeon (PhD Fall 2015, currently U.California Merced), Ali Rahnamoun (PhD summer 2016, currently Michigan State U.), Alireza Ostadhossein (PhD summer 2016, currently Stanford), Dr. Lili Gai (currently Mount Sinai, NY), Sungwook Hong (PhD summer 2016, currently U.Southern California), Kichul Yoon (PhD Fall 2016, currently at Agency for Defense Development, South Korea), Mahbub Islam (PhD Fall 2016, currently at Purdue U.), Dr. Mark Fedkin (Dutton Institute, Penn State), Dr. Roghayyeh Lotfi (Advanced Semiconductor Materials. Phoenix), ASM Jonayat (PhD summer 2018, currently at Intel), Abhishek Jain (PhD Fall 2019), Shabnam Sharmin (PhD Fall 2019, currently Oxford (UK)), Mert Sengul (PhD Spring 2020, currently U.Maryland), Chowdhury Ashraf (PhD Spring 2019, currently U. Washington), Seung Ho Hahn (PhD Summer 2020, currently Samsung), Dr. Chen Chen (currently Penn State), Behzad Damirchi (PhD June 2021, currently City of Hope, LA), Dooman Akbarian (PhD May 2021, currently NiH fellow), Kate Penrod (PhD June 2021), Aditya Lele (PhD, June 2021, currently Princeton University), Hyunguk Kwon (PhD June 2021, currently U.Pittsburgh, Jamil Hossain (PhD Oct 2021, currently Brown U.), Nabankur Dasgupta (PhD Oct 2021, currently Sandia National Lab), Yawei Gao (PhD Dec 2021, currently Oak Ridge National Lab), Karthik Ganeshan (PhD Oct 2021, currently Schrodinger Inc), Siavash Rajabpour (PhD Dec 2021, currently employed in Iran), Dr. Dundar Yilmaz (currently NextGen), Jessica Schulze (PhD March 2022, currently patent law), Mahdi Talkhoncheh (PhD April 2022, currently FDA), Kamyar Roshan (PhD April 2022, currently City of Hope), Ben Evangelisti (PhD April 22, currently unemployed), , Dr. Simon Delattre (currently Penn State), Dr. Swarit Dwivedi (currently Monash University), Dr. Nadire Nayir (currently U. Izmir, Turkey)

*Current graduate students*: Ga-Un Jeong, Emdadul Chowdhury, Yuwei Zhang, Mozhdeh Mirakhory, Mahmoud Mortazavi, Mengyi Wang, Alireza Sepehrinezhad

*Current postdoctoral staff*: Dr. Yun-Kyung Shin (Associate Research Professor), Dr. Malgorzata Kowalik (Associate Research Professor), Dr. Tao Wang (postdoc), Dr. Qian Mao (postdoc)