Aditya Dilip Lele

Email : adl233@psu.edu

EDUCATION

- **Pennsylvania State University** — State College, PA, USA
  Doctor of Philosophy in Mechanical Engineering; CGPA:3.93/4.0 — *Aug '18 – current*
  Doctoral minor in Computational Materials
- **Indian Institute of Technology Madras** — Chennai, India
  Master of Science (by research) in Mechanical Engineering; CGPA:8.8/10 — *Jan '16 – Jul '18*
- **Vishwakarma Institute of Technology** — Pune, India
  Bachelor of Technology in Mechanical Engineering; CGPA: 9.31/10 — *July '11 – May '15*

ACADEMIC EXPERIENCE

- **Postdoctoral research associate** — Princeton Uni., USA
  Advisor: Prof. Yiguang Ju — *Sept '21 – current*
  - Modeling non-equilibrium plasma catalysis
    - Understanding the effects of surface charging on adsorption energies
    - This could potentially explain synergistic plasma catalysis effects
  - Polymer decomposition
    - Large scale atomistic simulations of different polymers using ReaxFF to understand their pyrolysis
    - Information leveraged to perform experiments
  - Laminar flame speed measurement
    - Laminar flame speed measurement of 32 gasoline fuel mixtures using a Bunsen flame
  - Skills acquired : Multi-scale modeling, Flame speed measurement

- **Doctoral work: Applications of reactive molecular dynamics** — Penn State, USA
  Advisor: Prof. Adri van Duin — *Jan '19 – Sept' 21*
  - Combustion chemistry of renewable fuels
    - A standard framework is being developed using ReaxFF molecular dynamics simulations to study the combustion chemistry of existing as well as novel hydrocarbon fuels
    - This framework will be used to automate the generations of reaction mechanisms using reactive molecular dynamics simulations
  - Carbon materials
    - Large scale atomistic simulations of different fuels using ReaxFF to understand the underlying soot formation processes
    - Atomistic-scale simulations of CNT growth on metal nanoparticle surfaces in combustion synthesis
  - 2D Material synthesis
    - Atomistic-scale simulations and force field development for hBN growth on sapphire surfaces
    - Multi-scale simulations to understand CVD growth of hBN
  - Skills acquired : Reactive molecular dynamics, Plane wave and molecular orbital DFT, Reactive force field training, Accelerated MD

- **Master's work: Development of a surrogate mechanism for biodiesel** — IIT Madras, India
  Advisors: Dr. Krithika Narayanaswamy and Dr. Anand Krishnasamy — *Jan '16 – Jul '18*
  - Experimental measurements of pressure, temperature and NO_x are obtained in a CI engine to assess the correctness of the kinetic model description.
  - A well validated surrogate mechanism has been developed as a part of this project, which can be successfully employed in engine CFD studies to predict and understand NO_x formation.
  - Skills acquired : Combustion kinetic modeling, Model reduction, Engine CFD modeling

- **Research Internship: Ignition delay time measurement for Methyl Butanoate in RCM** — PTB, Germany
  Advisors: Prof. Ravi Fernandes and Dr. Kai Moshammer — *May '17 - July '17*
  - Ignition delay time measurements were performed in a single piston Rapid Compression Machine (RCM) to investigate auto-ignition behavior of methyl esters complementing surrogate mechanism development as a part of master's thesis project.
  - Skills acquired : Auto-ignition experimentation, pressure and temperature measurement

PUBLICATIONS

- **Lele, Aditya**, Lin, Ying and Yiguang Ju. A DFT study on the effect of surface charging on adsorption energies of N and H. **(*Under preperation*)**
- **Lele, Aditya**, and Adri CT van Duin. ReaxFF based modelling of soot formation in ethylene fuel rich conditions with force field enhancements. **(*Under preperation*)**
- Banerjee, R., Granzier-Nakajima, T., **Lele, A.**, Schulze, J., Hossain, M. J., Zhu, W., Pabbi, L., Kowalik M., van Duin, A. C. T., Terrones, M., & Hudson, E. W. On the origin of non-classical ripples in draped graphene sheets.
- Efstratios Kritikos, **Aditya Lele**, Adri C.T. van Duin, & Andrea Giusti. Reactive Molecular Dynamics Study of the Effects of an Electric Field on *n*- Dodecane Combustion. **(*Accepted in Combustion and Flame*) (*Under Review in ACS Applied Nano Materials*)**
- **Lele, Aditya**, Predrag Krstic, and Adri CT van Duin. "ReaxFF Force Field Development for Gas-Phase hBN Nanostructure Synthesis." The Journal of Physical Chemistry A (2022).
- Malgorzata Kowalik , Md Jamil Hossain , **Aditya Lele** , Wenbo Zhu , Riju Banerjee , Tomotaroh Granzier-Nakajima, Mauricio Terrones, E.W. Hudson , Adri C. T. Van Duin. Atomistic-scale simulations on graphene bending near a copper surface, Catalysts 2021, 11(2), 208.
- **Lele, A.***, Kwon, H*., Ganeshan, K., Xuan, Y., & van Duin, A. C. (2021). ReaxFF molecular dynamics study on pyrolysis of bicyclic compounds for aviation fuel. Fuel, 297, 120724.
- Kwon, Hyunguk*, **Aditya Lele***, Junqing Zhu, Charles S. McEnally, Lisa D. Pfefferle, Yuan Xuan, and Adri CT van Duin. "ReaxFF-based molecular dynamics study of bio-derived polycyclic alkanes as potential alternative jet fuels." Fuel 279 (2020): 118548.
- **Lele, Aditya**, Karan Soni, Krithika Narayanaswamy, and Anand Krishnasamy. Experimental and Modeling Investigation of NO Formation Mechanism for Biodiesel and Its Blend with Methanol. No. 2019-01-0217. *SAE Technical Paper*, 2019.
- **Lele, Aditya D.**, Sonal K. Vallabhuni, Kai Moshammer, Ravi X. Fernandes, Anand Krishnasamy, and Krithika Narayanaswamy. "Experimental and chemical kinetic modeling investigation of methyl butanoate as a component of biodiesel surrogate." *Combustion and Flame* 197 (2018): 49-64.
- Vallabhuni, Sonal K., **Aditya D. Lele**, Vaibhav Patel, Arnas Lucassen, Kai Moshammer, Mohammed AlAbbad, Aamir Farooq, and Ravi X. Fernandes. "Autoignition studies of Liquefied Natural Gas (LNG) in a shock tube and a rapid compression machine." Fuel 232 (2018): 423-430.
- **A. D. Lele**, K. Anand, K. Narayanaswamy, Surrogates for biodiesel: review and challenges, in: Biofuels A. Agarwal, R. Agarwal, T. Gupta, B. Gurjar (Eds), Biofuels, Green Energy and Technology, Springer, Singapore, 2017, pp. 177-199.

**Joint first author*

CONFERENCES AND POSTERS

- **Aditya Lele**, Simon Delattre, Margaret Kowalik, and Adri CT van Duin. "Application of machine learning to extrapolate reactive molecular dynamics simulation results to experimental and engineering-relevant time scales.", IndustryXchange poster session (2020), The Pennsylvania State University.
- **Aditya Lele**, Kwon, Hyunguk, Junqing Zhu, Charles S. McEnally, Lisa D. Pfefferle, Yuan Xuan, and Adri CT van Duin. "ReaxFF-based molecular dynamics study of bio-derived polycyclic alkanes as potential alternative jet fuels.", Future of Bioenergy and Biorenewables poster session (2020), The Pennsylvania State University. **(3rd place prize)**
- **A. D. Lele**, K. Anand, K. Narayanaswamy, Development of a chemical kinetic mechanism for biodiesel surrogate, 10 th US National Combustion Meeting (2017), Paper 2D02.

PROFESSIONAL EXPERIENCE AND CERTIFICATIONS

- **Essentials of Online Teaching**
  Pennsylvania State University — *Fall 2020*
- **Eaton India Pvt. Ltd.**
  Project: Gear shift quality assessment tool development in MS Excel — *Jul '15 – Dec '15*
- **Panse Autocomp Pvt. Ltd.**
  Internship Project: Single minute exchange process of die for manufacturing automobile components. — *May '13 – Jul '13*

TECHNICAL SKILLS

- **Simulation tools:** FlameMaster, ChemKin, Forte, ReaxFF, LAMMPS, Gaussian, VASP
- **Programming Languages:** C++, Perl
- **Other:** Linux, LaTeX, MS Excel, MATLAB

TEACHING EXPERIENCE

- **Teaching assistant:** Indoor Air Quality Engineering (Penn State, Fall 2018), Numerical Methods for Thermal Engineering (IIT Madras, Spring 2017)
- **Mentoring:** Mentored an undergraduate intern on "Fuel surrogate optimization" project

SCHOLASTIC ACHIEVEMENTS

- Received "Indo-German Centre for Sustainability" scholarship for a short term research stay in Germany, 2017.
- Received HTRA (Research Assistantship) for the entire duration of M.S. degree
- One among 750 students from a pool of about 350,000 students to be awarded National Talent Search Examination Scholarship by the Government of India, 2008
- 9^{th} state rank in High school Scholarship exam by State Government of Maharashtra, 2006.

REFERENCES

- Doctoral advisor: Prof Adri van Duin, Penn State. (acv13@psu.edu)
- Master's advisor: Prof Anand Krishnasamy, IIT Madras. (anand_k@iitm.ac.in)
- Course instructor: Prof Michael J. Janik, Penn State. (mjj13@psu.edu)