



DELAWARE ENERGY
INSTITUTE



Transforming Process Industries

VIRTUAL KINETICS LAB

REACTION SOFTWARE ECOSYSTEM

ONLINE WORKSHOP

***TOOLS TO ACCELERATE MULTISCALE
MODELING WORKFLOW***

WORKSHOP AGENDA

Monday - Dion Vlachos: *Multiscale Modeling and VLab*

Overview

Tuesday - Gerhard Wittreich: *Reaction Mechanisms;*

pMuTT – python Multiscale Modeling Toolbox

Wednesday- Gerhard Wittreich: *pGrAdd – python Group*

Additivity; python demos for pMutt and pGrAdd



WORKSHOP AGENDA

Thursday – *OpenMKM* – *Open-source Microkinetic*

Modeling; ReNView – *Reaction Network Viewer; petBOA*

– *Parameter Estimation with Bayesian Optimization*

Friday - *Chemical Kinetics Database; NEXTorch* – *Next*

Experiment Toolkit in PyTorch; AIMSIM + *Astartes* –

Artificial Intelligence Molecular Similarity + *Astartes*



DION VLACHOS

UNIDEL DAN RICH CHAIR IN ENERGY PROFESSOR OF CHEMICAL & BIOMOLECULAR ENGINEERING

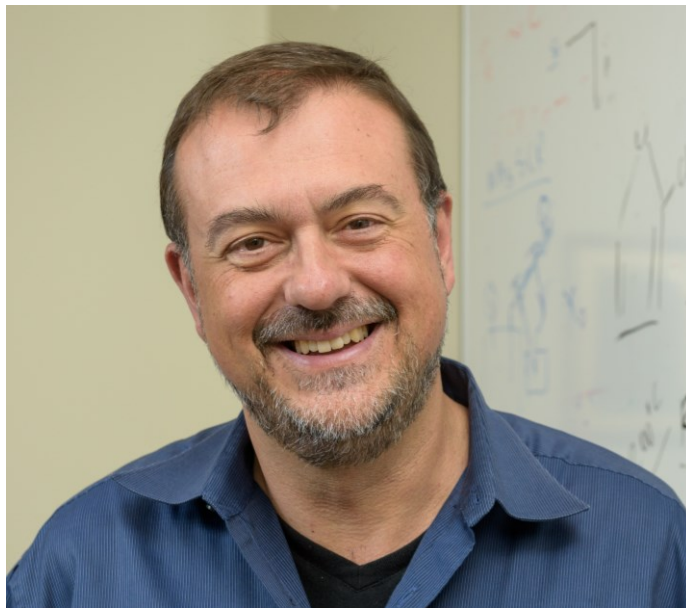
UNIVERSITY OF DELAWARE

Director: Delaware Energy Institute

Catalysis Center for Energy Innovation

Center for Catalytic Science & Technology

Monday: *Multiscale Modeling and VLab Overview*



GERHARD WITTREICH

RESEARCH SCIENTIST

UNIVERSITY OF DELAWARE

AIChE Board Member

P.E.; Ph.D. University of Delaware

Tuesday: *Reaction Mechanisms; pMuTT – python
Multiscale Modeling Toolbox*

Wednesday: *pGrAdd – python Group Additivity;
python demos for pMutt and pGrAdd*



SASHANK KASIRAJU

COMPUTATIONAL SCIENTIST

UNIVERSITY OF DELAWARE

Ph.D. University of Houston

Thursday: OpenMKM – Open-source

Microkinetic Modeling

petBOA - Parameter Estimation with Bayesian
Optimization



UDIT GUPTA

SOLUTIONS ARCHITECT

SIEMENS DIGITAL INDUSTRIES SOFTWARE

Ph.D. University of Minnesota

Thursday: ReNView – *Reaction Network Viewer*



SIDDHANT LAMBOR

COMPUTER SOFTWARE ENGINEER

UNIVERSITY OF DELAWARE

M.S. Carnegie Mellon University

Friday: [CKineticsDB](#) – *Chemical Kinetics
Database*



YIFAN WANG

RESEARCH SCIENTIST

META

Ph.D. University of Delaware

Friday: NEXTorch - *Next Experiment Toolkit
in PyTorch*



JACKSON BURNS

DEPARTMENT OF ENERGY COMPUTATIONAL SCIENCE GRADUATE FELLOW

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
B.C.H.E. Honors University of Delaware

Friday: AIMSIM + astartes - Artificial
Intelligence Molecular Similarity + Astartes



VLACHOS GROUP

PROFESSOR DION VLACHOS

RESEARCH ASSOCIATE DIRECTORS

SCIENTIFIC RESEARCH STAFF

POSTDOCTORAL RESEARCHERS

GRADUATE STUDENT RESEARCHERS

UNDERGRADUATE STUDENTS

INTERNS



ZOOM CHAT Q & A

CHAT MODERATORS

DION VLACHOS

SASHANK KASIRAJU

SIDDHANT LAMBOR



SLACK CHANNEL

SLACK MODERATORS

VLACHOS GROUP

SCIENTIFIC RESEARCH STAFF

POSTDOCTORAL RESEARCHERS

GRADUATE STUDENT RESEARCHERS



VIDEO RECORDINGS

VLAB WEBSITE

https://dei.udel.edu/vlab_workshop



GITHUB

VIRTUAL KINETICS LAB

<https://github.com/VlachosGroup>



