2019 UD-ANL WORKSHOP

NOVEMBER 21, 2019

University of Delaware

Argonne National Laboratory

GROUP 1

Saleem Ali
Neil Sturchio
Anouar Benali
Matthew Otten

Industrial Ecology and linkages to Argonne Polymer Lifecycle Research

Saleem H. Ali

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Energy and the Environment

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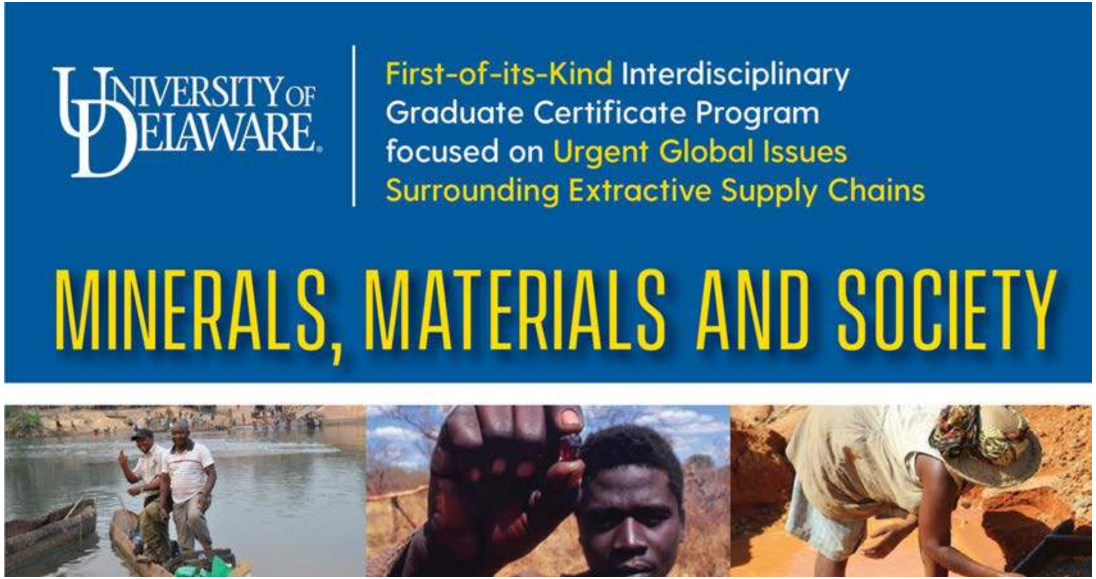
Research Areas and Linkages

- Life Cycle Analysis Comparisons between Metals and Polymers
- How can innovative materials (particularly polymers) facilitate the transition towards a “circular economy” with greater emphasis on upcycling?
- What are the rebound effect implications of particular material usage and pricing?
- The role of polymers in meeting the 17 Sustainable Development Goals (particularly SDG 12)
- Synergies with my roles as a member of the United Nations IRP and the GEF’s Scientific and Technical Advisor Panel

Case studies and teaching content delivery



Interfacial processes under confinement: Microfluidics and X-ray Imaging at APS

Research Team:
Neil Sturchio & Bektur Abdilla - UD Earth Sciences
Jason Gleghorn & Ali Bozorgnezhad – UD Biomedical Engineering
Paul Fenter, Sang Soo Lee & Irene Almazan - ANL Chem. Sci. & Engineering

Approach:

Combine UD's expertise in microfluidics with ANL's expertise in advanced synchrotron X-ray scattering and imaging methods to explore new frontiers in solid-liquid interface processes and emergent behavior under confinement.

Importance:

This research has potential impact in a broad range of applications including fundamental understanding of solid-liquid interfacial processes; underground storage of nuclear waste and CO_2; extraction of hydrocarbons and geothermal energy; fabrication of complex nano-patterned materials

Team Strengths

- UD (Gleghorn and colleagues) has extensive experience in developing microfluidics and nanofluidics for biomedical applications, and in 2018 a collaboration was initiated (with Sturchio and Abdilla) in geochemical applications

- ANL (Fenter and colleagues) and UD (Sturchio) have existing collaboration involving synchrotron X-ray scattering studies of solid-liquid interfaces and have discussed extending collaboration to in situ microfluidics studies

- Availability of new synchrotron beamlines at ANL and NSLS-II that are suitable for advanced in-situ microfluidics experiments, in conjunction with in-house studies to be performed at UD

Anouar Benali,
Computational Science Division
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DIFFUSION MONTE CARLO FOR HIGH ACCURACY SIMULATIONS OF MOLECULES AND SOLIDS

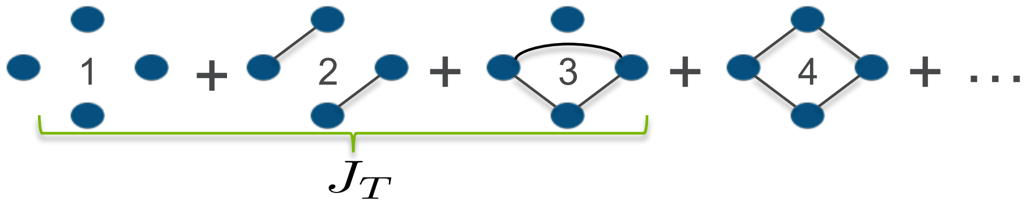
Wavefunction Ansatz

$$\Psi = e^{J}\Phi_T$$

exchange/static correlation: antisymm., orbital-based

"(dynamic) correlation"

J:



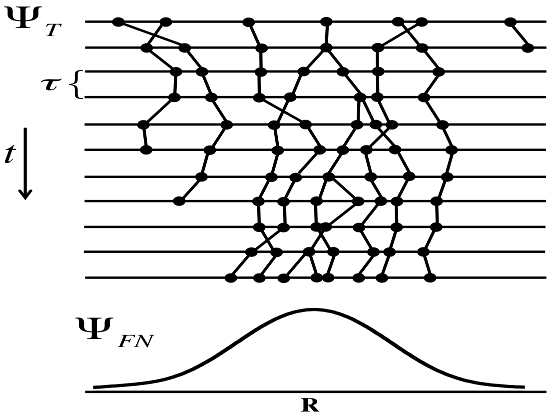
Imaginary Time Projection

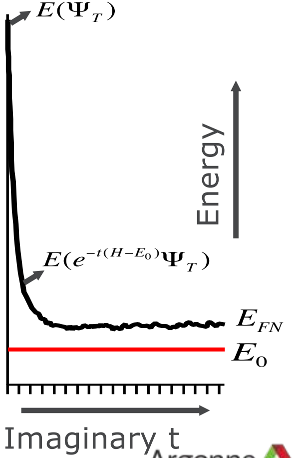
$$e^{-t(\hat{H}-E_0)}\Psi_T \xrightarrow[t\to\infty]{} e^{J_{DMC}}\Phi_T$$

$$\hat{H} = -\tfrac{1}{2}\nabla^2 + V_{ee} + V_{eI} + V_{II} + V_{FN} + (\Psi_T^{-1}V_{eI}\Psi_T - V_{eI})$$

Fixed node constraint	Pseudopotential Localization

Source of uncontrolled errors

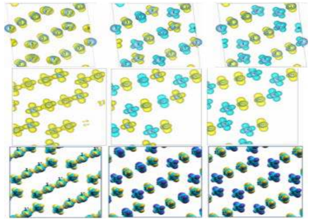


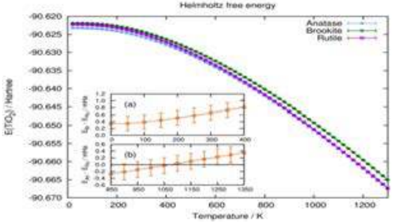


APPLICATION TO MATERIAL SCIENCE AND QUANTUM CHEMISTRY

Anouar Benali, benali@anl.gov

Stability of TMO (Ti_4O_7 / TiO_2, NiO etc..)





Energy barriers in catalysis (Pt surfaces)

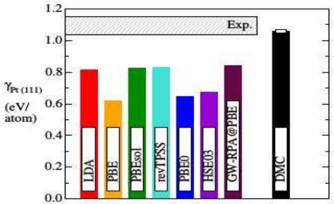
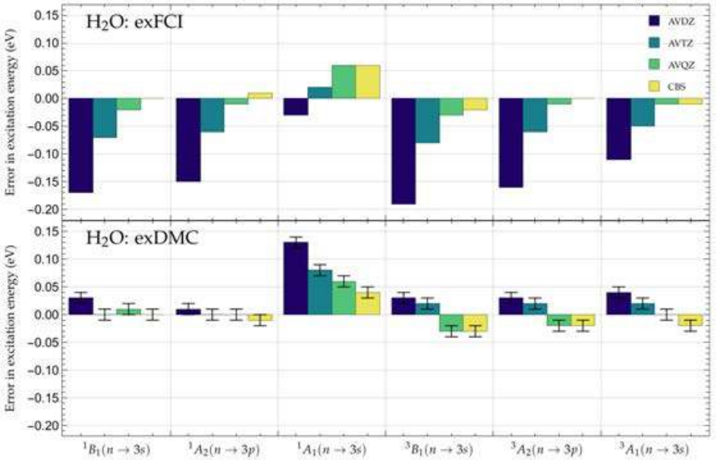
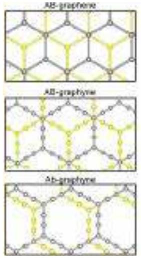


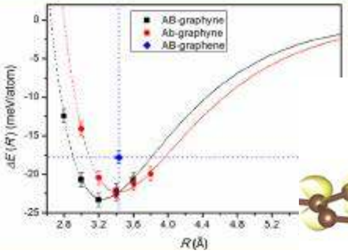
Figure 3: Pt(111) surface energy computed using Diffusion Quantum Monte Carlo (DMC) and other electronic structure methods, including hybrid (HSE03) DFT and RPA calculations [43, 44]. The DMC agrees with experiment within the *experimental* uncertainty. The white bar indicates the statistical error of the DMC.

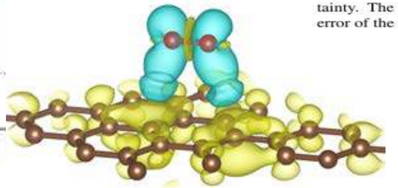
Excited States in Molecules



Properties of van der Waals bi-layered materials







Metal Organic Framework (Barrier energies)

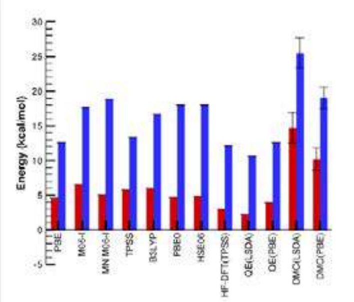
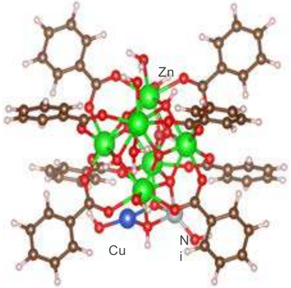
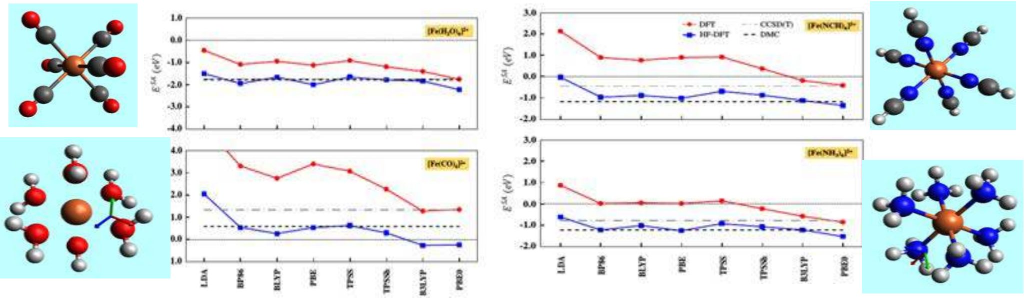


FIG. 1. Energy barriers in kcal/mol for ethylene hydrogenation with E(TS)-E(R) in red, and E(P)-E(TS) in blue; the error bars on the DMC values are ± one standard deviation.

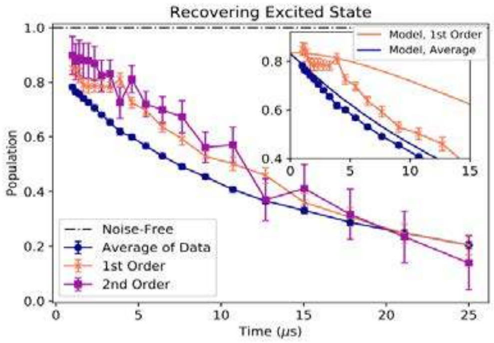


Benchmarking new DFT methods



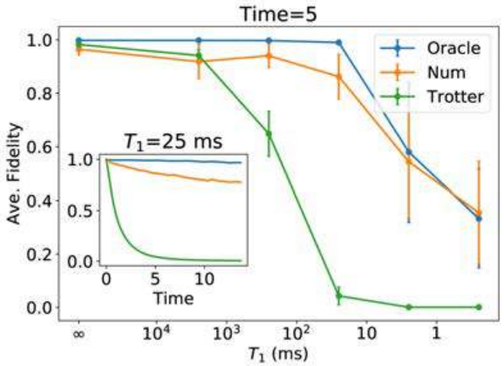
Theory and Modeling for Controllable Quantum Systems

Matthew Otten, Maria Goeppert Mayer Fellow, ANL, otten@anl.gov



- QuaC – Parallel, general open quantum systems solver
  - quantum dot/plasmon, electron bubble systems, phonon bath cooling, error mitigation in quantum circuits, bosonic quantum information processing…

- Development of Algorithms and Error Mitigation Methods



  - Error mitigation through noise extrapolation
  - Hybrid quantum dynamics algorithms
  - New spectroscopy methods based on QIS
  - New quantum machine learning kernels
  - Verification and validation of quantum computers

GROUP 2

Ganesh Sivaraman
Javier Garcias-Frias
Vishal Saxena
Yuping Zeng

UD-ANL WORKSHOP (2019)

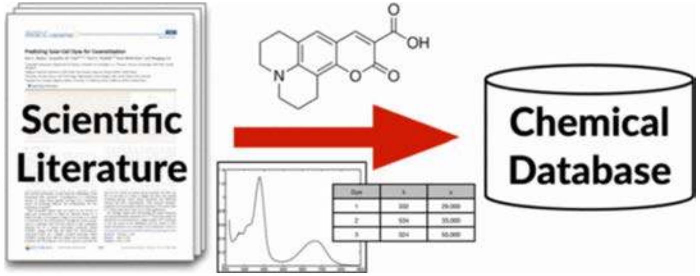
Argonne NATIONAL LABORATORY

SIMULATION, DATA, AND LEARNING DRIVEN MATERIALS INFORMATICS

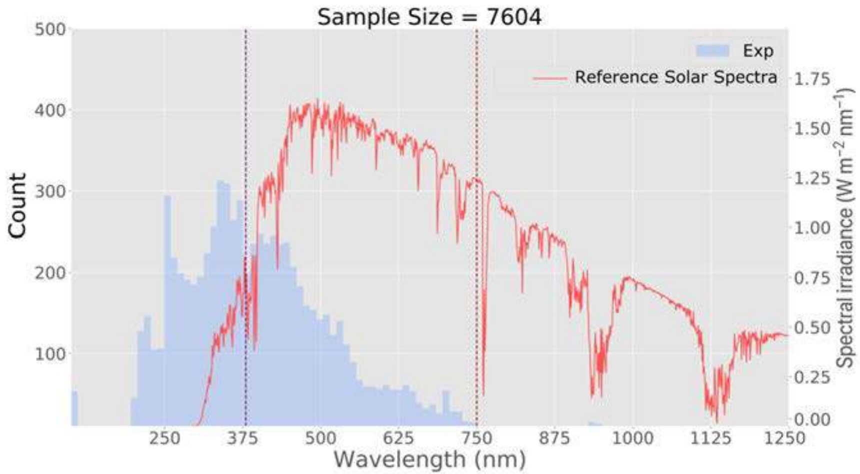
GANESH SIVARAMAN
Postdoctoral Appointee
Argonne Leadership Computing Facility
EMAIL: gsivaraman@anl.gov

November 21 (2019)

NATURAL LANGUAGE PROCESSING DRIVEN MATERIAL DISCOVERY [1]



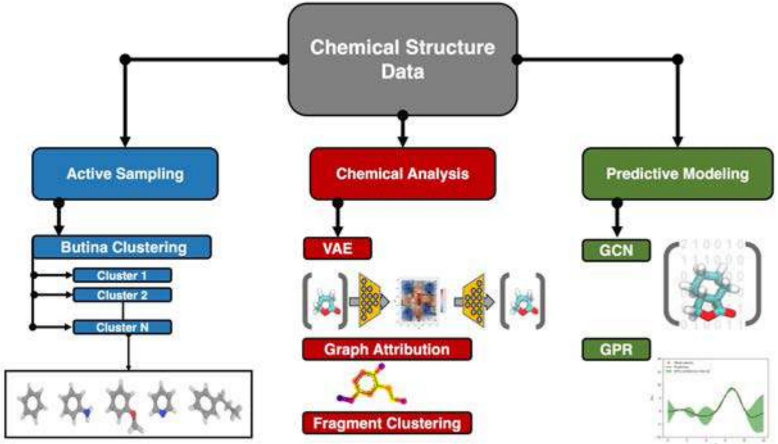
- NLP driven quantum chemistry workflow applied to an initial corpus of ~ **400,000** scientific literature.



[1] http://chemdataextractor.org/

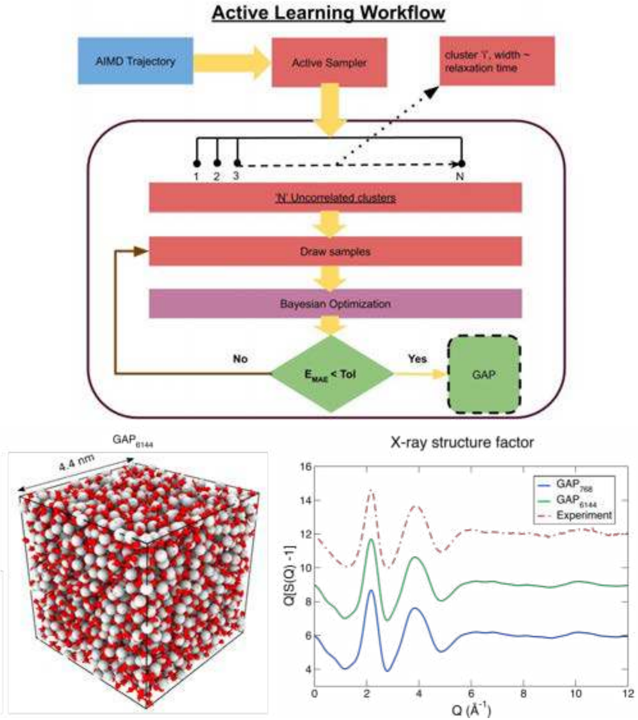
E. J. Beard,G. Sivaraman, Á. Vázquez-Mayagoitia, V. Vishwanath, J. M. Cole, ***Comparative dataset of experimental and computational attributes of UV/vis absorption spectra***, Sci. Data. (Accepted)

Molecular Melting Points



Sivaraman *et. al.*, ***A diversified machine learning strategy for predicting, and understanding molecular melting points***" (Preprint: 10.26434/chemrxiv.9914378.v1).

Automating ML Forcefield Generation



Sivaraman *et. al.*, ***Machine Learning Inter-Atomic Potentials Generation Driven by Active Learning: A Case Study for Amorphous and Liquid Hafnium dioxide*** (Preprint: arXiv:1910.10254).

THANK YOU!

QUESTIONS?

This research used resources of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC02-06CH11357.

Graph-Based Quantum Stabilizer Codes

Javier Garcia-Frias
ECE Department

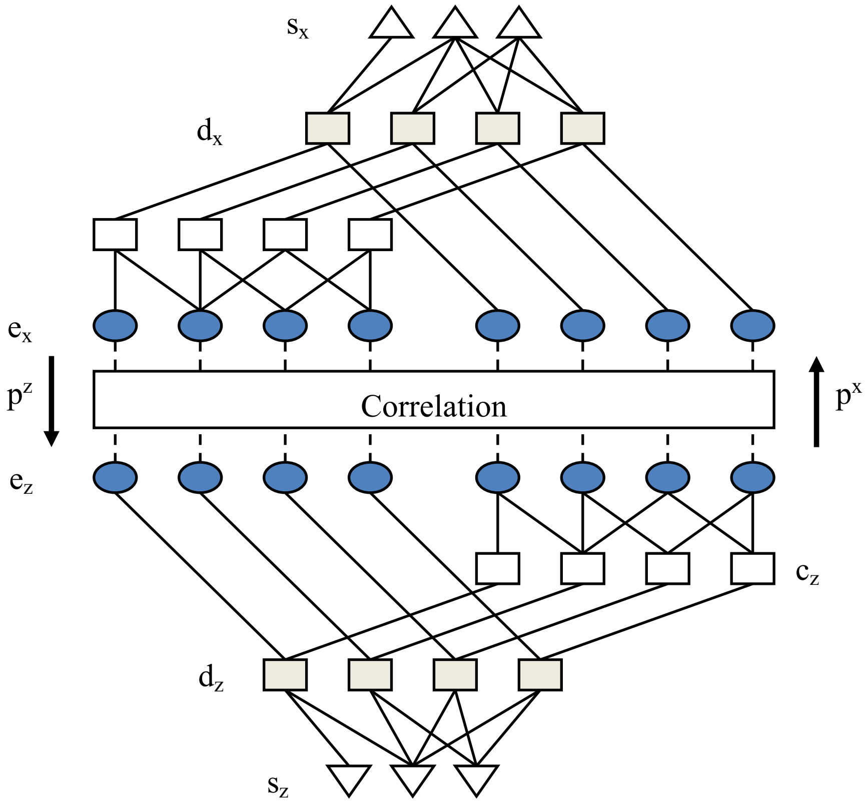
Research interests
Graph-based channel coding exploiting channel/source statistics

Stabilizer Codes

- Quantum operators for one-qubit described by 2-by-2 complex unitary (Pauli) matrices
  - Bit flip: $X(\alpha|0\rangle+\beta|1\rangle)=\alpha|1\rangle+\beta|0\rangle$
  - Phase flip: $Z(\alpha|0\rangle+\beta|1\rangle)=\alpha|0\rangle-\beta|1\rangle$
  - Combination of bit and phase flip: $Y(\alpha|0\rangle+\beta|1\rangle)=i\alpha|1\rangle-\beta|0\rangle$
- Stabilizer codes
  - A set of Pauli operators, $\{S_i\}$, on N qubits. Any two stabilizers commute with each other
  - Quantum codeword, $|\psi\rangle$: +1 eigenstate of all the stabilizer generators: $S_i|\psi\rangle=S_i$ for all i
- Error operator, E_α
  - Pauli operator taking a quantum state to a (possibly) corrupted state: $|\psi\rangle \rightarrow E_\alpha|\psi\rangle$
- Syndrome of E_α, s
  - "Commutation status" (either commute or anti-commute) of E_a with respect to all the stabilizers
  - Only measurement from physical system
- Representation as classical code
  - Write stabilizers as row in matrix $A=(A_1|A_2)$: Eg., XIYZ=-(XIXI) x(IIZZ)=-(1010|0011)
  - Commutativity of stabilizers $\rightarrow A_1A_2^T+A_2A_1^T=0$
  - Represent E_α as a binary string, e_a, of 2N bits, reversing the order to the X and Z operators Eg., XIYZ=-(XIXI) x(IIZZ)=(0011|1010)

Problem reduces to classical coding: Obtain most likely e_α so that $s=Ae_\alpha$

Implementation and Research Topics



- Decoding performed using message passing in corresponding graph
  - Analytical tools to predict performance
  - Closed-form expressions of error floors
- Quantum channel statistics (depolarizing channel, channels with memory) can be included in decoding graph.
- Sometimes channel parameters can be estimated jointly with the decoding process
- Goal: Subject to constraint $A_1A_2^T+A_2A_1^T=0$, design graphical structure (matrix A) to optimize performance
- Results:
  - CSS LDGM-based codes
  - Non-CSS stabilizer LDGM-based codes

Sustaining Advances in Integrated Circuits Research

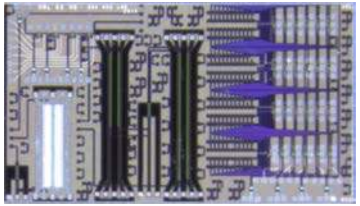
Dr. Vishal Saxena, Associate Professor

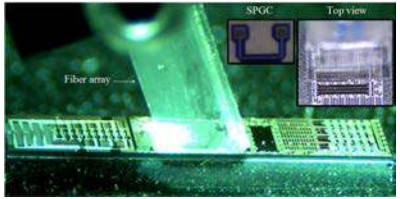
Electrical and Computer Engineering Dept, Email: vsaxena@udel.edu

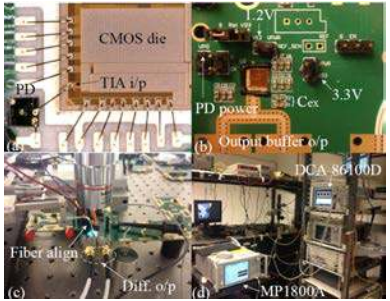
Analog Mixed-Signal and Photonic Integrated Circuits (AMPIC) Lab

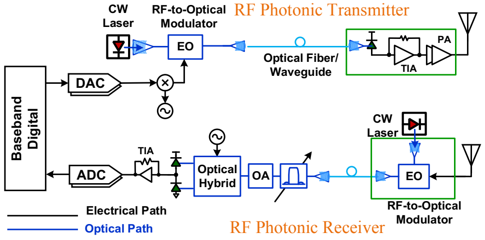
Hybrid Electronic-Photonic Integrated Circuits

- CMOS Photonic ICs for Terabit/s Optical Interconnects
  - Advanced Modulation Transceivers
- RF and Millimeter-wave Photonic ICs
- New Applications: Optical Quantum Computing & Machine Learning





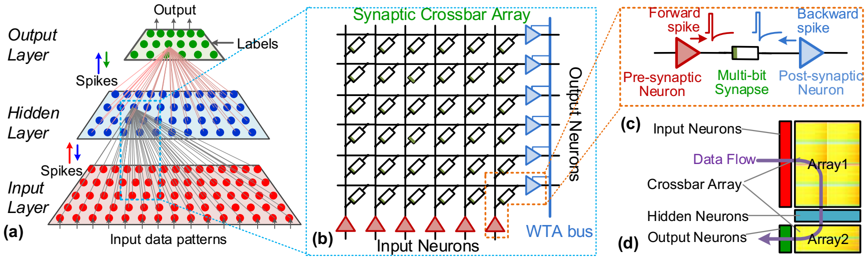


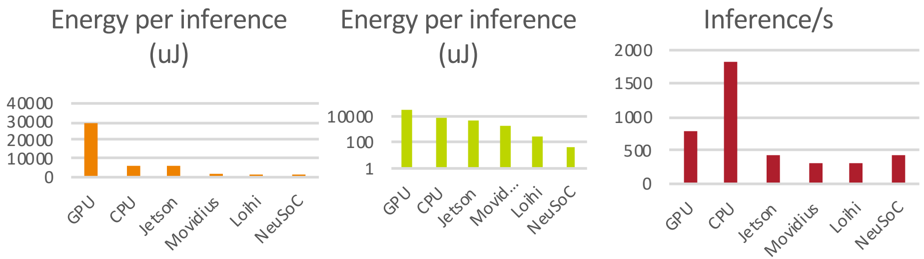


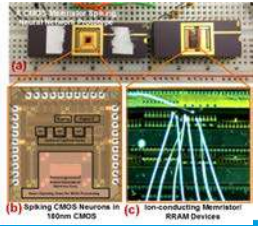
AMPIC Lab Research Overview

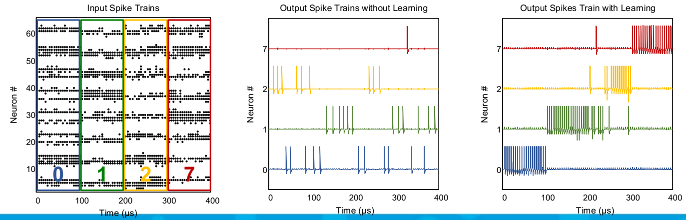
Neuromorphic Computing & Edge-AI

- Neuromorphic Computing using emerging memory devices
  - Portable Edge-AI hardware
  - Approach density and energy-efficiency of biological brains
  - Resistive RAM arrays integrated with CMOS neurons
- Spike-based NN learning algorithms
  - Algorithms to enable continuous learning with small amount of data
  - Semi-supervised learning









Advanced Compound Semiconductor Devices

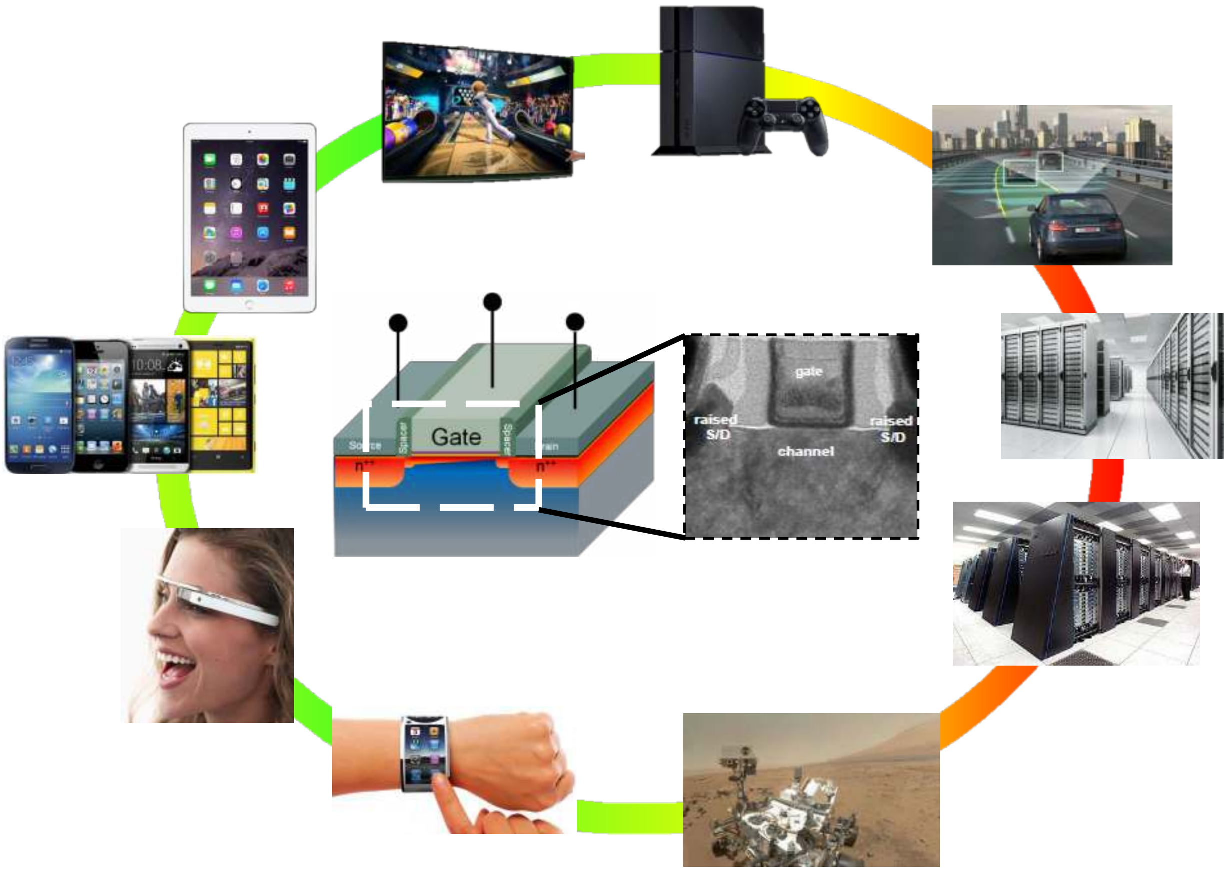
PI: Yuping Zeng (Assist. Prof.)

Department of Electrical & Computer Engineering

University of Delaware

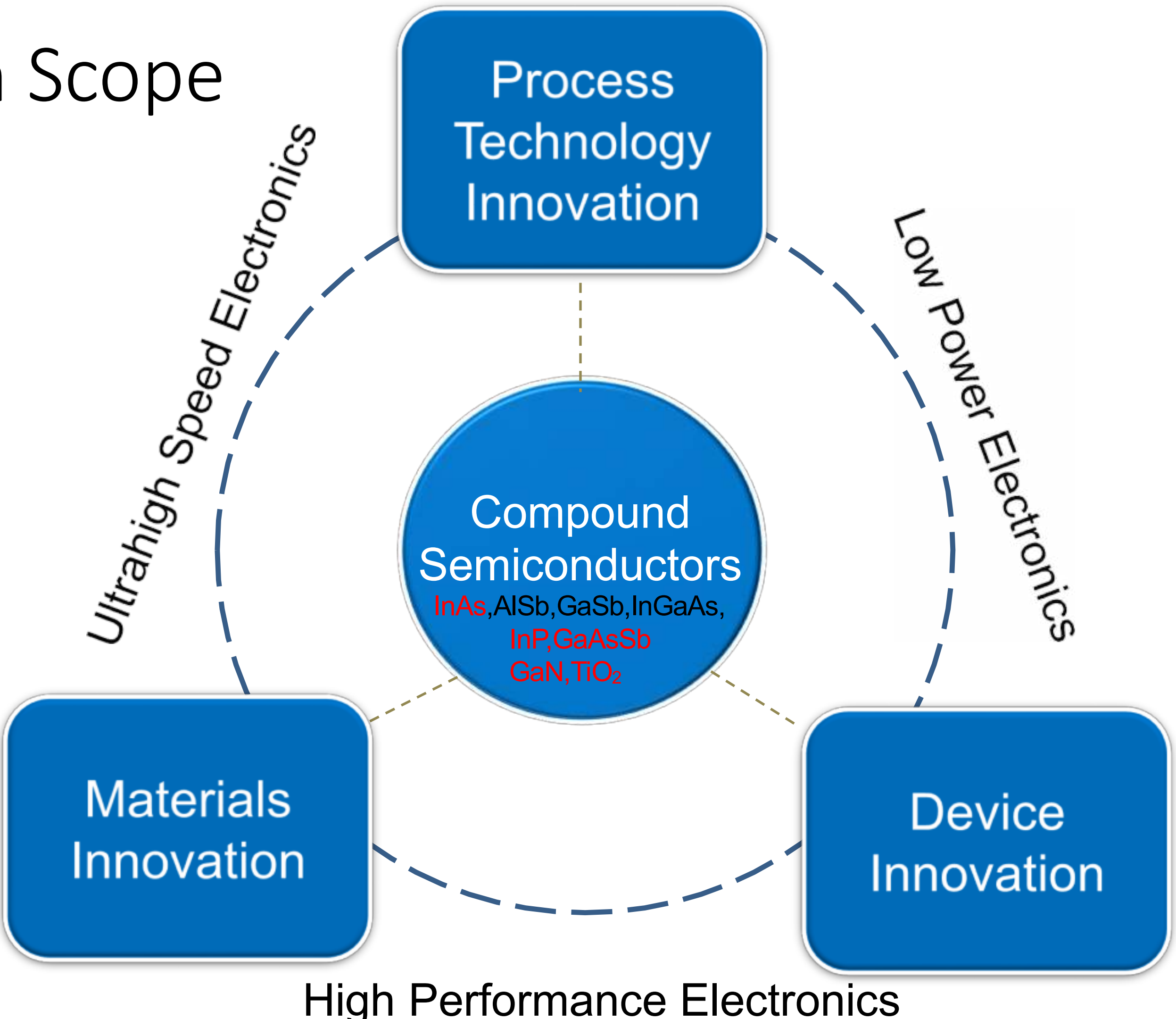
Nov 21, 2019

THE TRANSISTORS

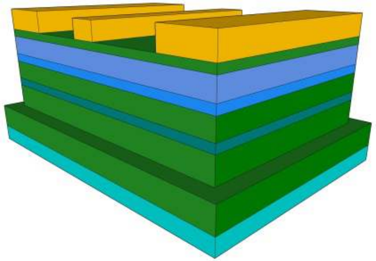


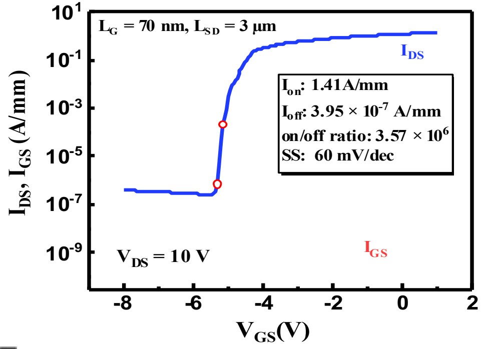
Billions of transistors switching billions of times a second to perform complex logic.

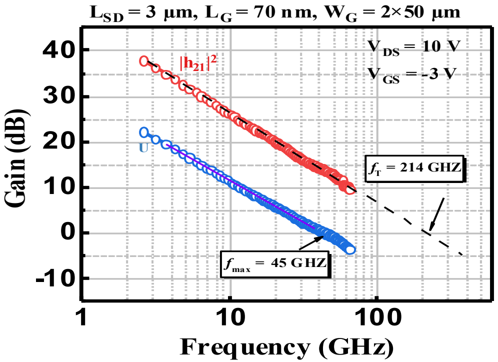
Research Scope

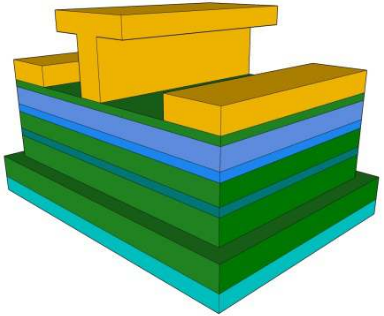


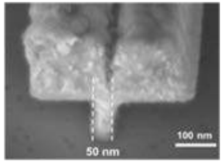
1. GaN-on-Si high electron mobility transistors



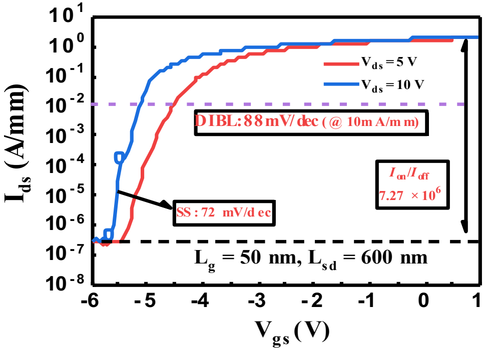


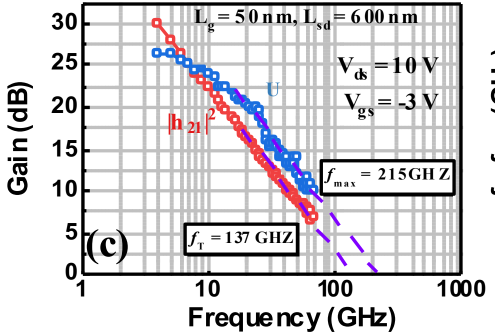






All are record values !

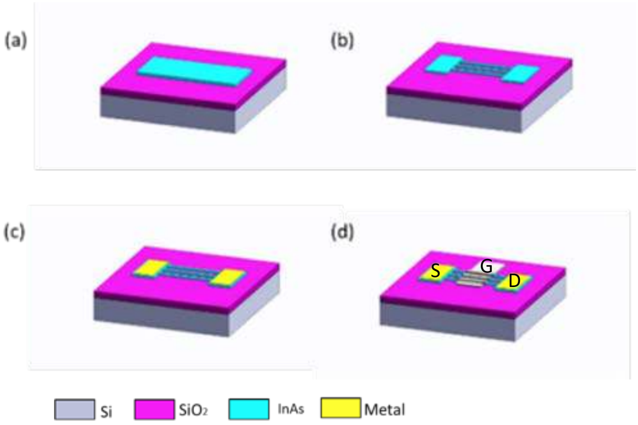


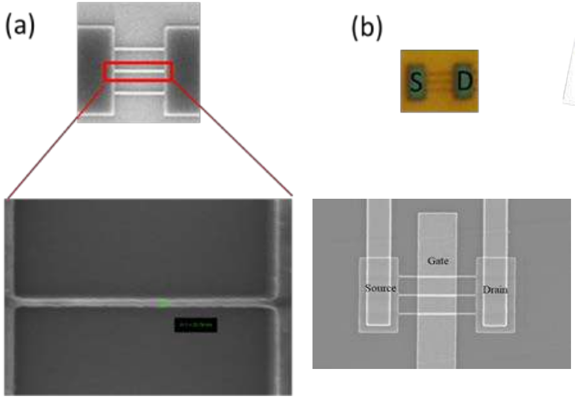


P Cui, Y Zeng et al, Applied Physics Express, 2019

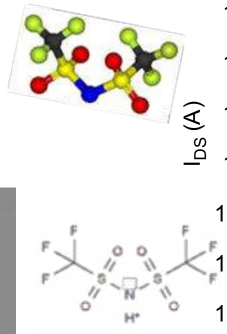
2. InAs fin field effect transistors

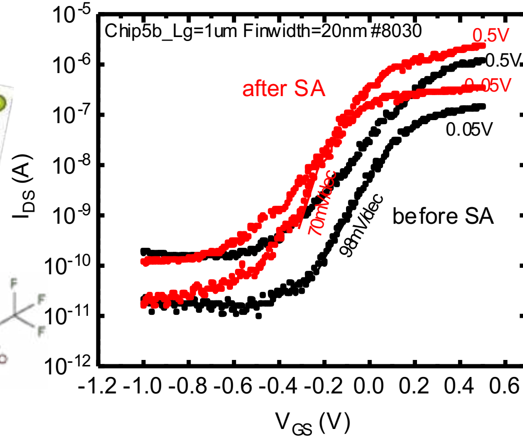
Fabrication process of InAs FinFETs





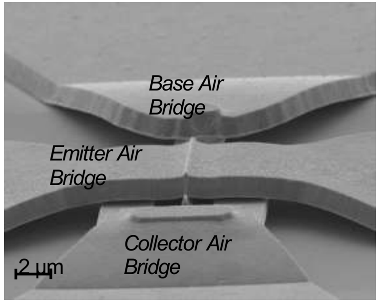
Super acid



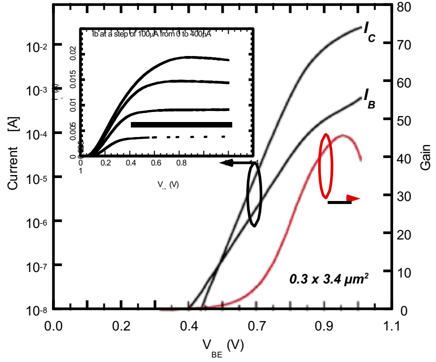


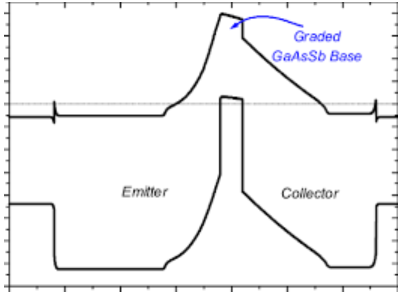
Y Zeng et al, IEEE Transaction on Electron Devices, 2019

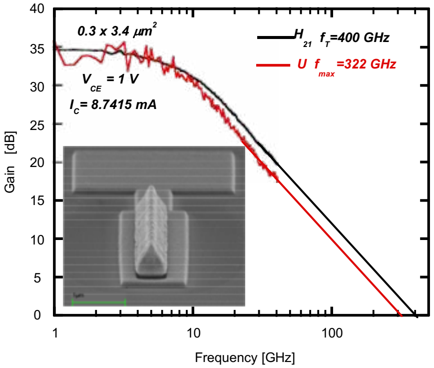
3. High speed heterojunction bipolar transistors



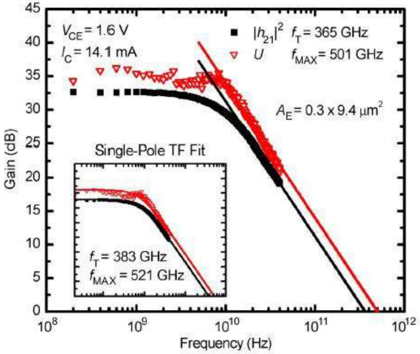
DC







RF



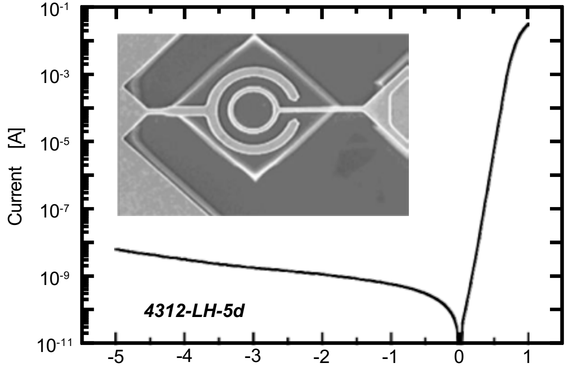
RF

InP/GaAsSb Heterojunction bipolar transistors

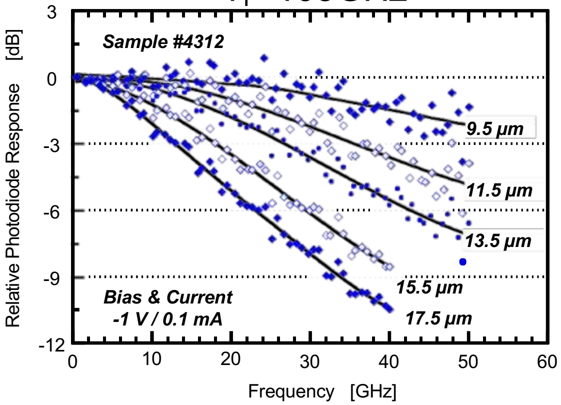
4. High speed unitravelling carrier photodiode

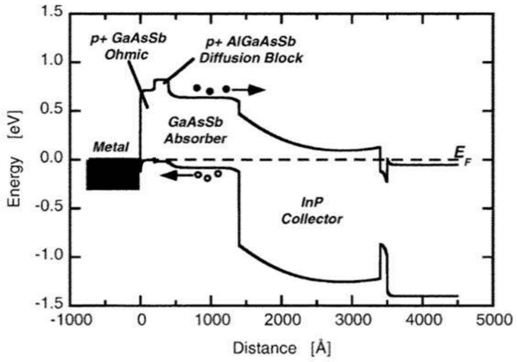
InP/GaAsSb Unitravelling carrier photodiode

Dark current

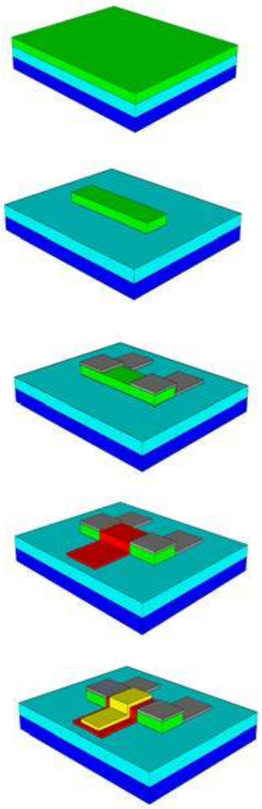


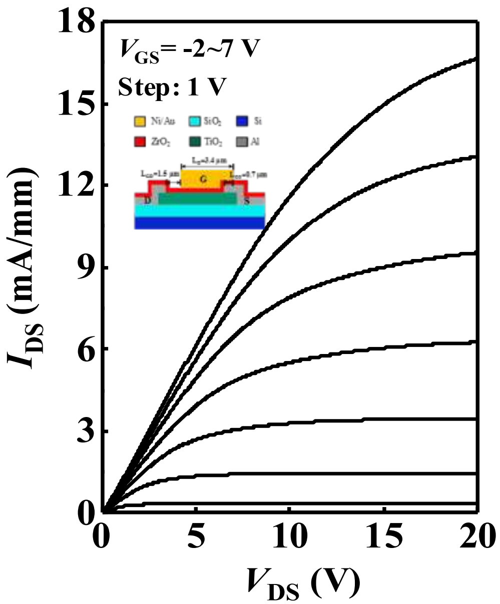
f_T=105GHz

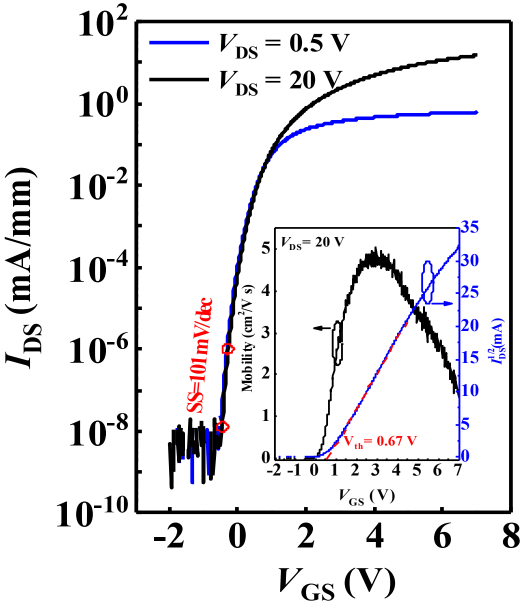




5. High performance TiO_2 thin film transistors







Record high I_{on} of 16.7 mA/mm, a record high I_{on}/I_{off} of 1.2×10^9 and a record low SS of 101 mV/dec.

Jie Zhang, Y Zeng et al, IEEE Electron Device Letters, 2019

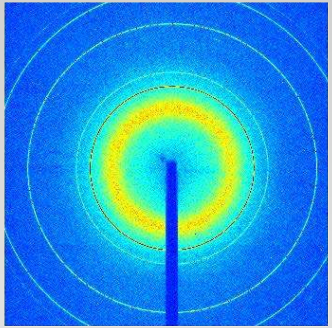
Ni/Au SiO_2 Si TiO_2 ZrO_2 Al

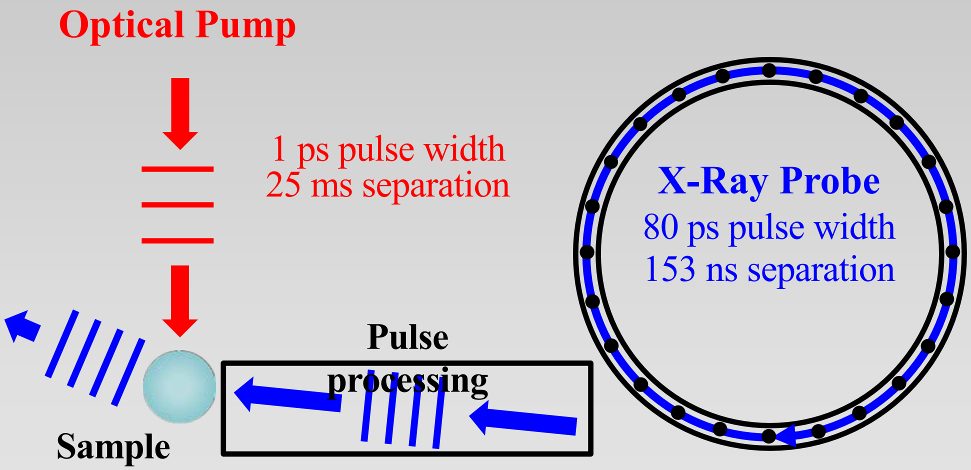
GROUP 3

Karl Unruh
Branislav Nikolic
Swati Singh

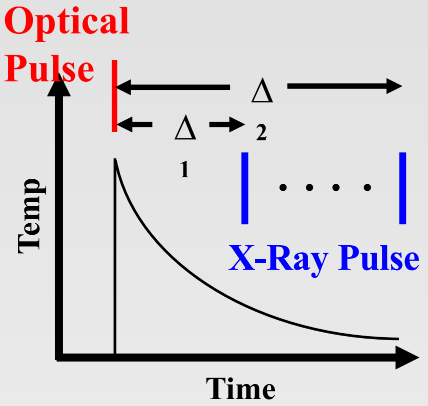
Ultrafast Optical Pump/X-Ray Probe Measurements at the APS

K.M. Unruh (DPA), M.F. DeCamp (DPA), K.H. Theopold (DCB), A.D. DiChiara (APS)





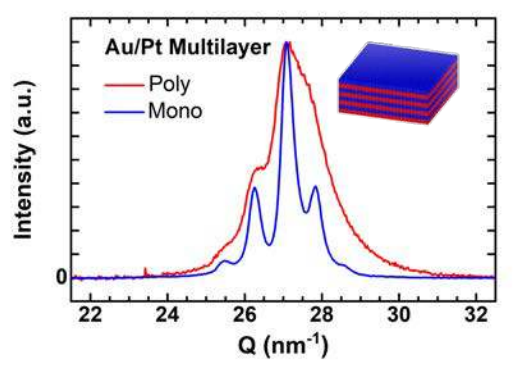
Advanced Photon Source Argonne National Laboratory



But there's a complication…

Monochromatic Beam → High Res./Low Intensity

Polychromatic Beam → Low Res./High Intensity

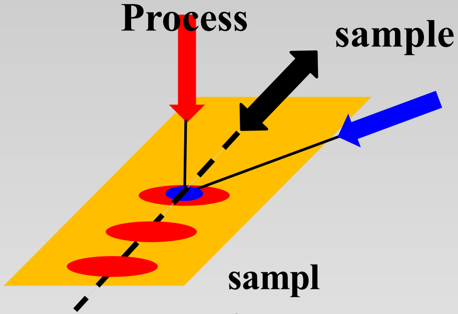


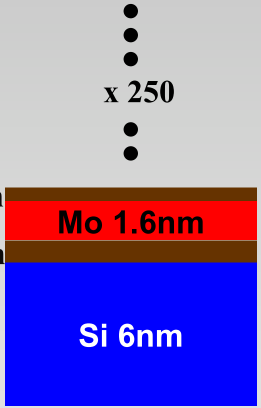
Ultrafast Optical Pump/X-Ray Probe Measurements at the APS

Reversible vs Irreversible Processes/Measurement optimization

Reversible Process

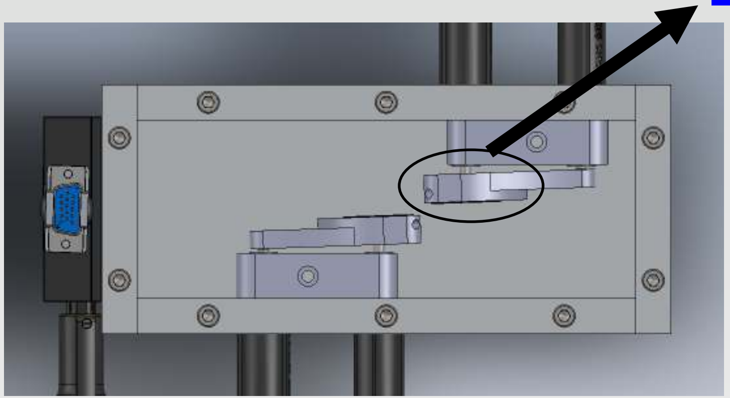
Irreversible Process



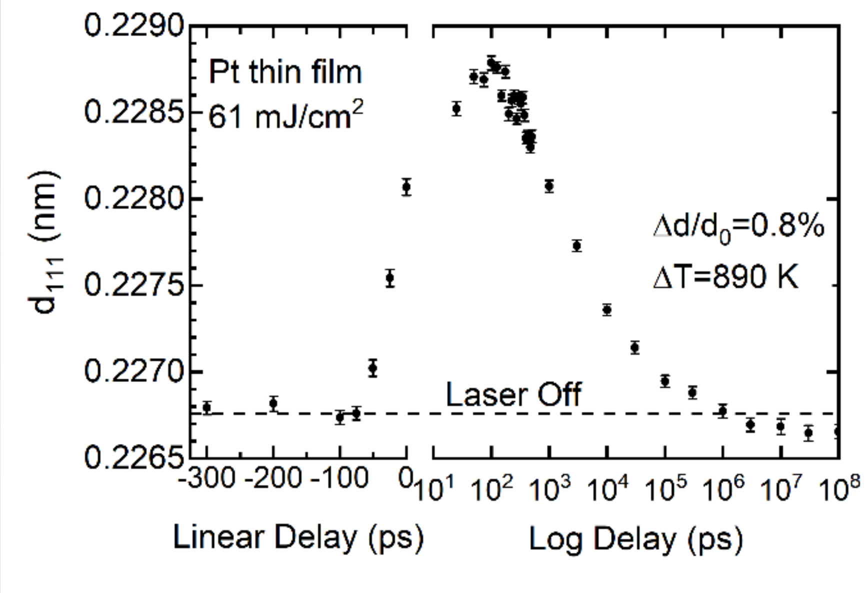


Ray Conley
APS

A tunable monochrometer



Derrick Allen
UD/DPA



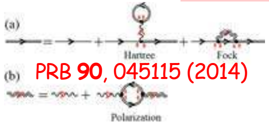
Thanks

NSF

Advanced Photon Source

Theoretical and Computational Quantum Transport for Nanostructures Far From Equilibrium

FORMALISMS



PRB **90**, 045115 (2014)

strong coupling to leads → NEGF

density of available quantum states:

$$G^r_{\sigma\sigma'}(t,t') = -\frac{i}{\hbar}\Theta(t-t')\langle\{\hat{c}_{\mathbf{r}\sigma}(t), \hat{c}^\dagger_{\mathbf{r}'\sigma'}(t')\}\rangle$$

how are those states occupied:

$$G^<_{\sigma\sigma'}(t,t') = \frac{i}{\hbar}\langle\hat{c}^\dagger_{\mathbf{r}'\sigma'}(t')\hat{c}_{\mathbf{r}\sigma}(t)\rangle$$

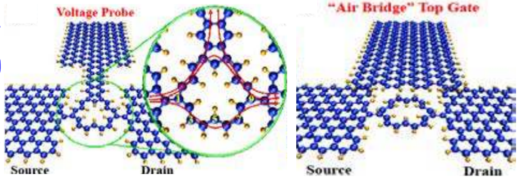
in elastic transport limit equivalent to Landauer-Büttiker scattering theory

weak coupling to leads → QME

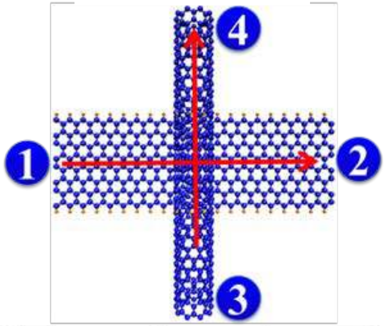
$$\begin{aligned} i\hbar\frac{d\hat{\rho}^I(t)}{dt} &= [\hat{H}^I_T, \hat{\rho}^I(t)] \\ \hat{\rho}_S &= \mathrm{Tr}_{\mathrm{leads}}[\hat{\rho}^I(t)] \end{aligned}$$

SYSTEMS

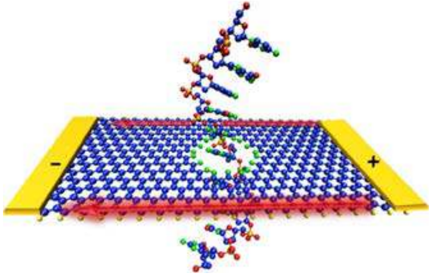
Molecular Electronics
PRL **105**, 236803 (2010)



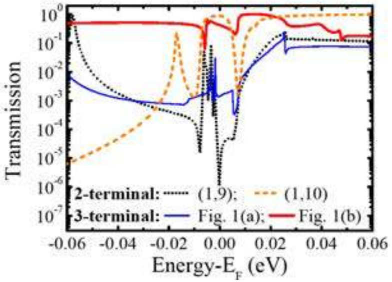
Nanoelectronics
JCEL **12**, 542 (2013)

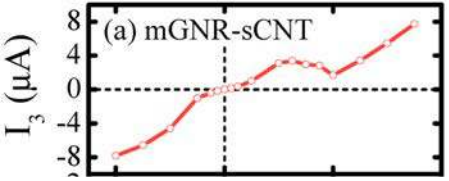


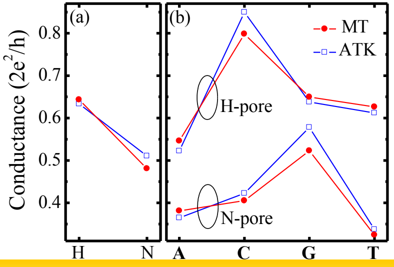
Nano-Bio Interface
Nano Lett. **12**, 50 (2012)



RESULTS

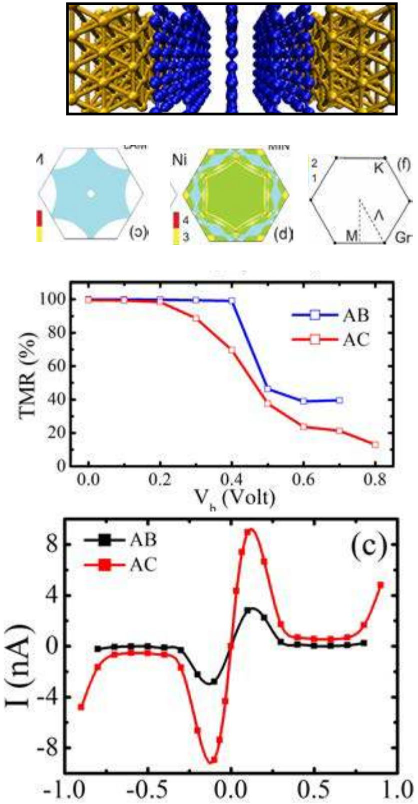




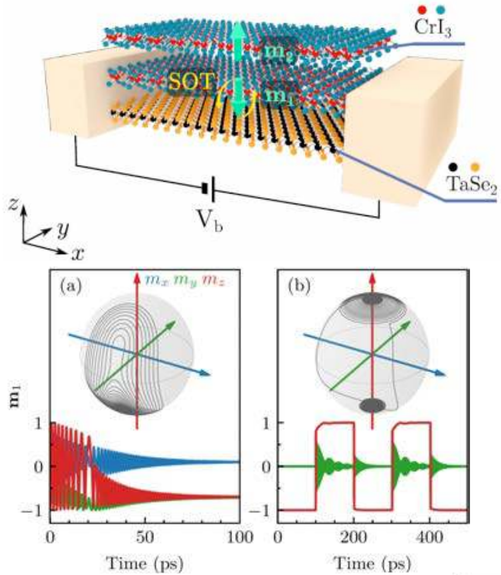


First-Principles or Time-Dependent Quantum Transport for Spintronics

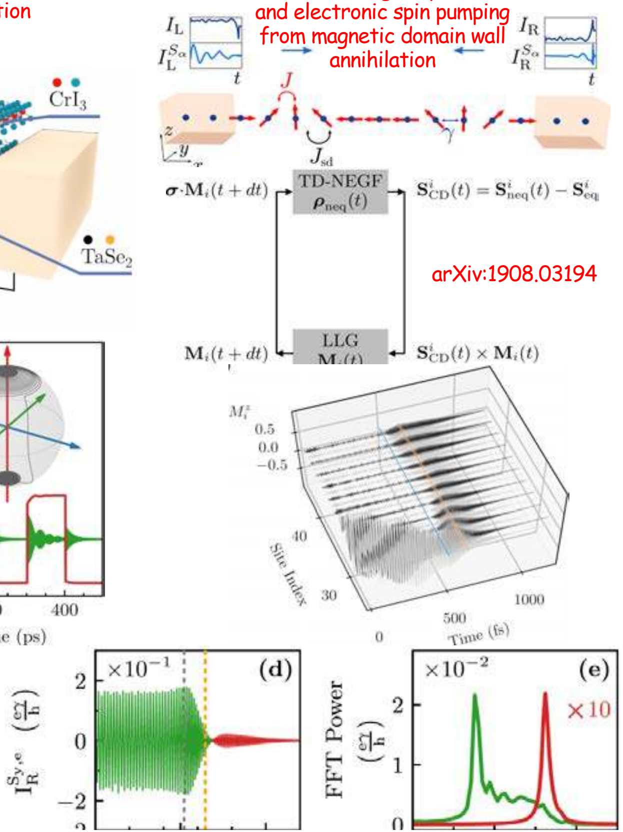
Colossal tunneling magnetoresistance
PRB. **85**, 184426 (2012)



Current-driven antiferromagnet-ferromagnet nonequilibrium phase transition in 2D magnets
arXiv:1909.13876

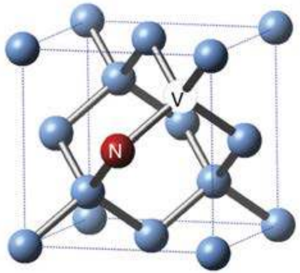


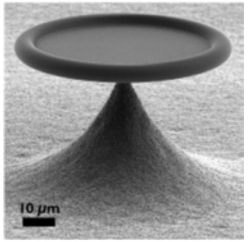
Short wavelength spin waves and electronic spin pumping from magnetic domain wall annihilation

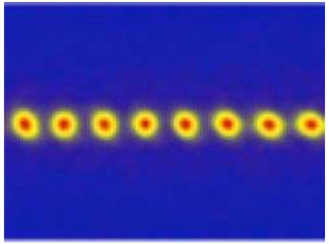


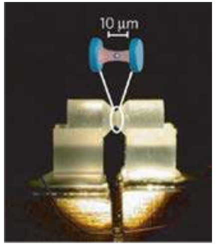
arXiv:1908.03194

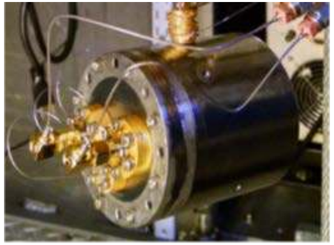
Quantum systems as sensors











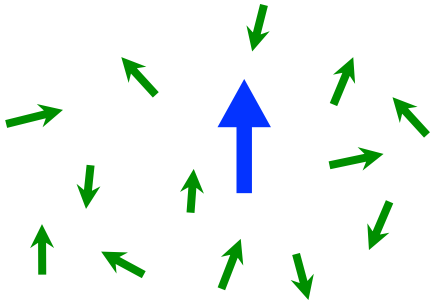
Bad qubits are excellent sensors of their environment!

- Could we use isolated quantum systems as precise measurement devices for classical forces and fields?
- Could we use quantum features (dark states, coherences, QND measurements) in these systems to make better sensors?
- Could we use controllable quantum systems as a testbed for exploring foundational physics questions?

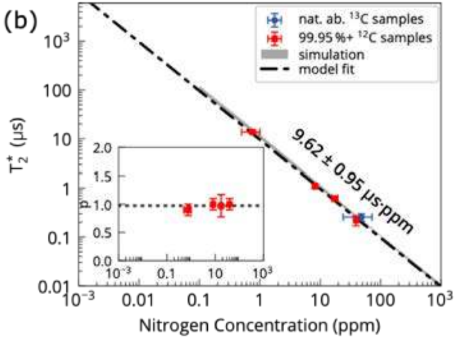
Quantum Spin based sensors

Developing pedagogical models for decoherence dynamics in various qubits and spin based sensors

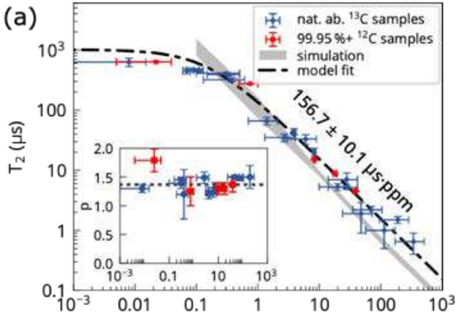
- cold atoms
- NV centers, quantum dots



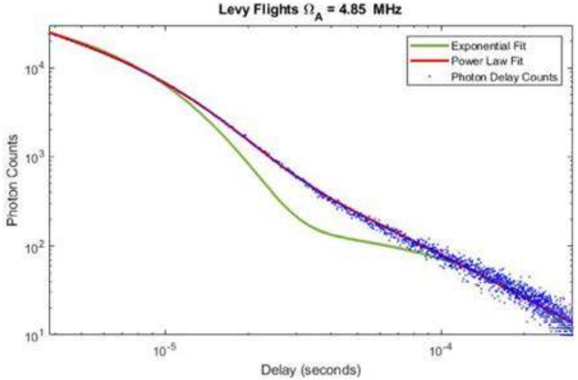
Recent work: decoherence in NV centers



E. Bauch et. al, Phys. Rev. X **8**, 031025 (2018).



E. Bauch, S. Singh et. al, [arXiv:1904.08763](https://arxiv.org/abs/1904.08763).

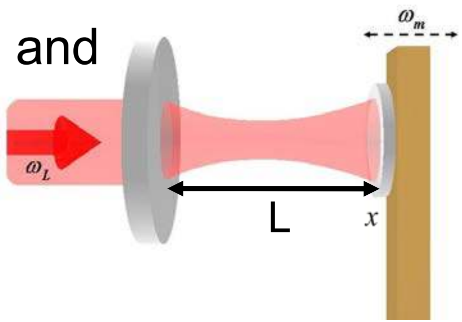


D. Levonian, M. Goldman, K. De Greve, S. Singh, S. Yelin, and M. Lukin, In preparation (2019).

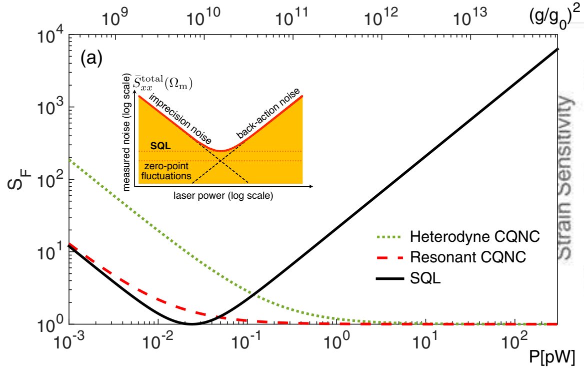
Optomechanical systems based sensors

Investigating mechanical systems as sensors of weak forces and quantum noise issues that limit them

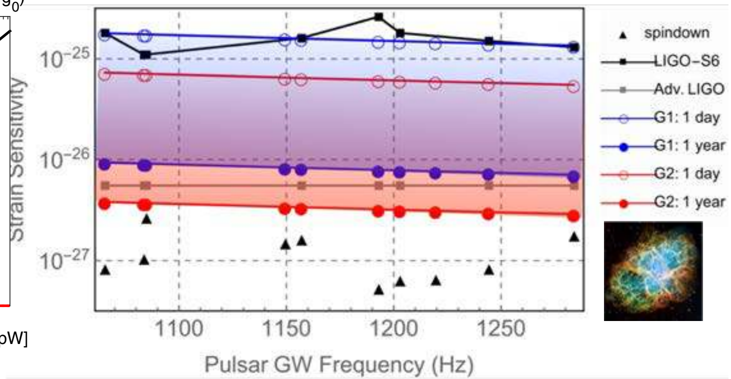
- astrophysical phenomena sensors
- quantum regime of mechanical systems



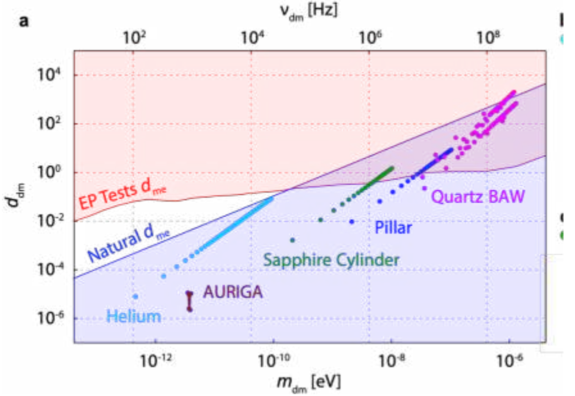
Recent work: backaction noise cancelation, pulsar GW and dark matter detection



F. Bariani, H. Seok, S. Singh, M. Vengalattore, P. Meystre, Phys. Rev. A 92, 043817 (2015).



S. Singh, L.A. DeLorenzo, I. Pikovski, and K.C. Schwab, New J. Phys. 19, 073023 (2017).



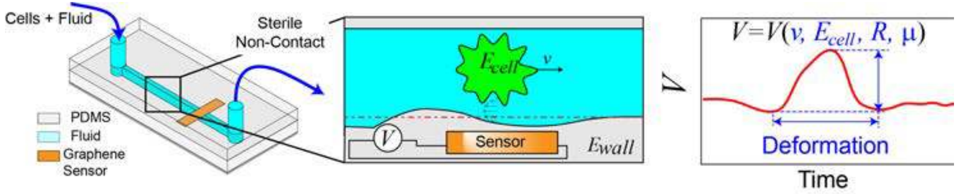
J. Manley, D. J. Wilson, R. Stump, D. Grin and S. Singh, arXiv1910.07574 (2019).

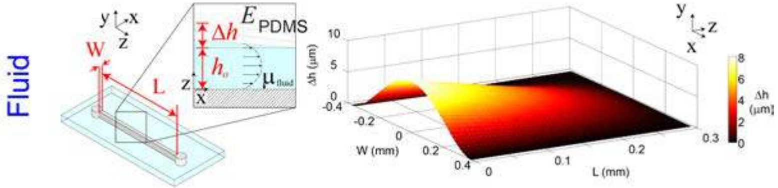
GROUP 4

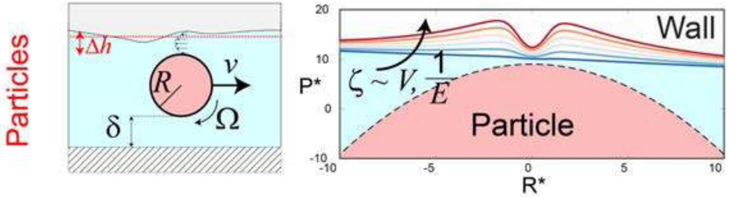
Charles Dhong
Kun Fu
Benjamin Gould
David Kaphan

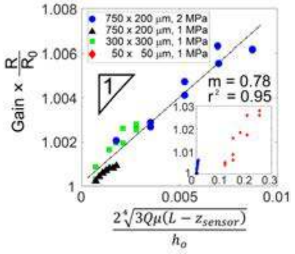
Mechanical Forces
at
Soft and Patterned Interfaces

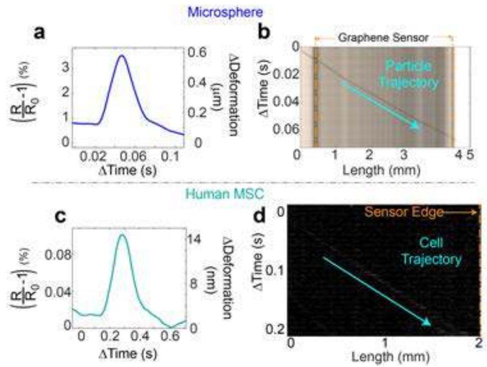
Dhong Lab
University of Delaware
Material Science &
Engineering
Biomedical Engineering











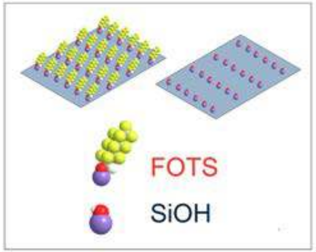
Experimental Platform for:

1. Elastohydrodynamic interactions in flow
2. Direct force measurements on thin films/membranes
3. Multiphysics in arbitrary channel geometries

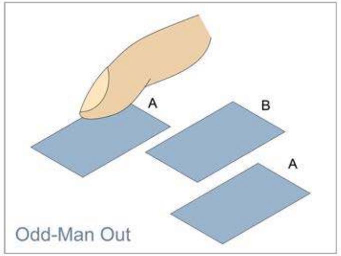
Dhong et al. *Nano Letters* 2018

Recreating Realistic Tactile Sensations

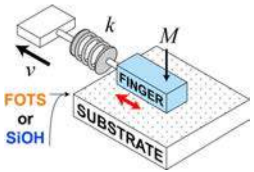
Reconfigurable Materials + Friction Mechanics + Perception

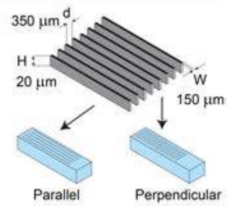


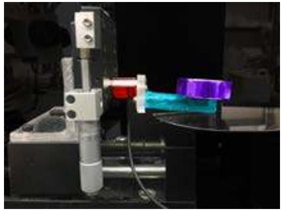
Single Molecule Haptic Discrimination

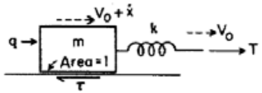


80% accuracy in humans (n =15)

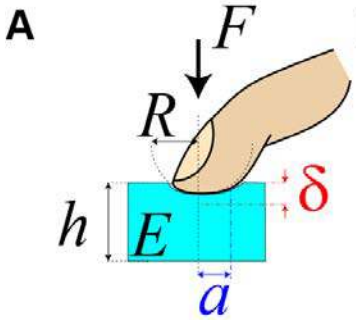


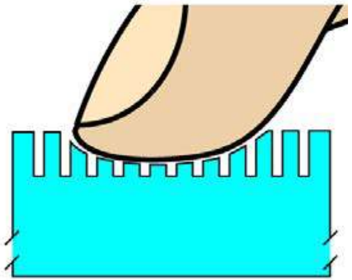






Stick-slip friction





"Which is Softer?"
(Two-alternative Forced Choice)

- Softness is measurable and preserved between subjects

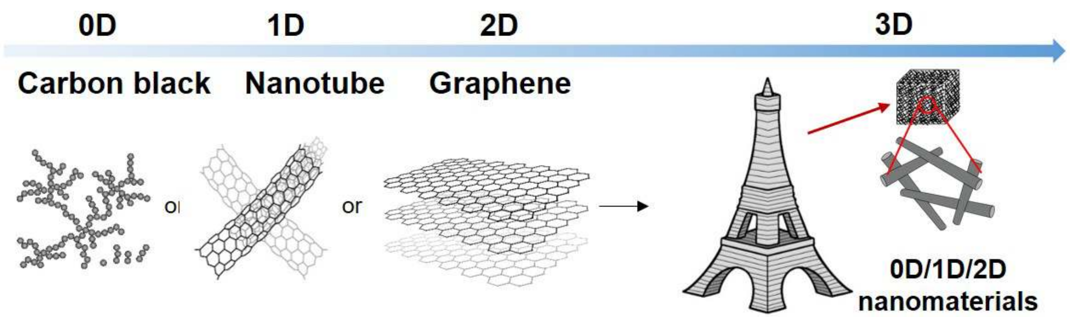
$$Softness = -8.4 + 1127\,[m^{-\frac{1}{2}}]\sqrt{\delta} + 1.8{\times}10^{6}\,[m^{-2}]\pi a^{2}$$

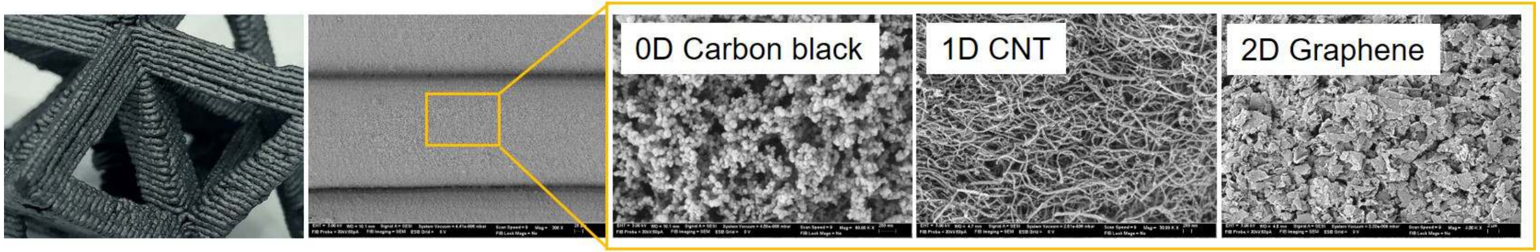
Dhong et al. *Soft Matter* 2018
Dhong et al. *Science Advances* 2019

Scalable additive manufacturing of 3D architectures with 0D/1D/2D materials

Kun (Kelvin) Fu
Assistant Professor
Mechanical Engineering
Center for Composite Materials
University of Delaware
kfu@udel.edu
www.kfu-group.com

Additive manufacturing of 3D architectures with 0D/1D/2D materials





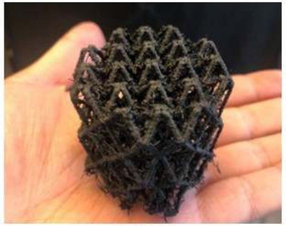
Examples:

Carbon black

Graphene

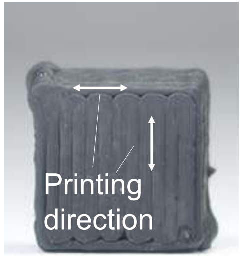
Graphene

CNT

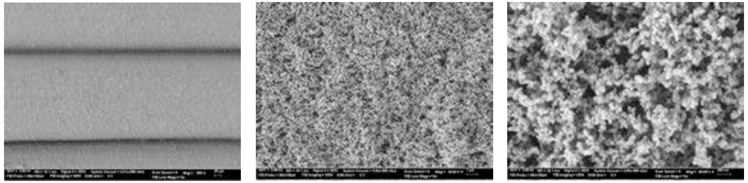


CNT

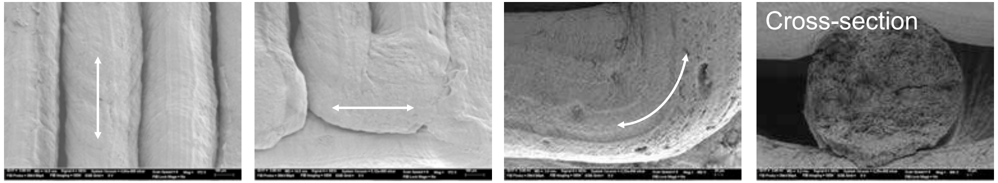
CNT



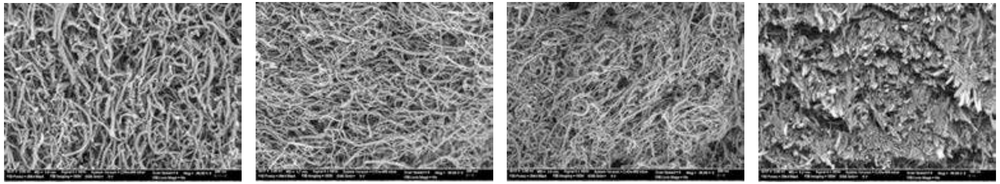
Homogeneously distributed carbon black



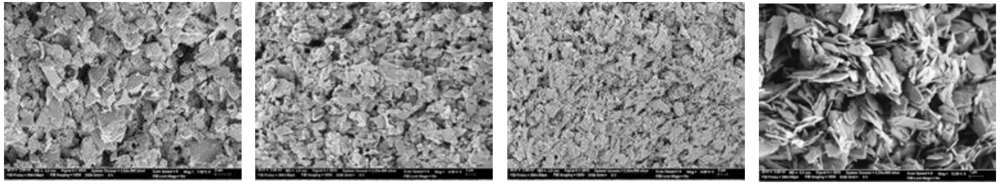
Filament printing direction



Highly aligned carbon nanotubes

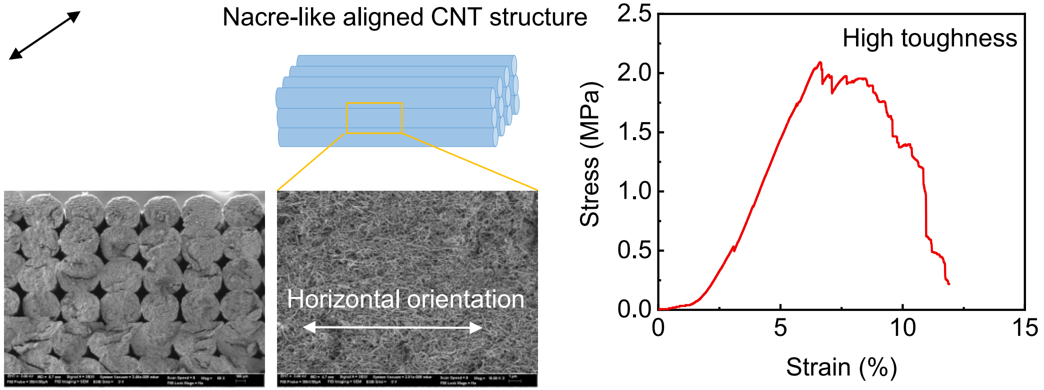


Highly aligned graphene nano-pallets

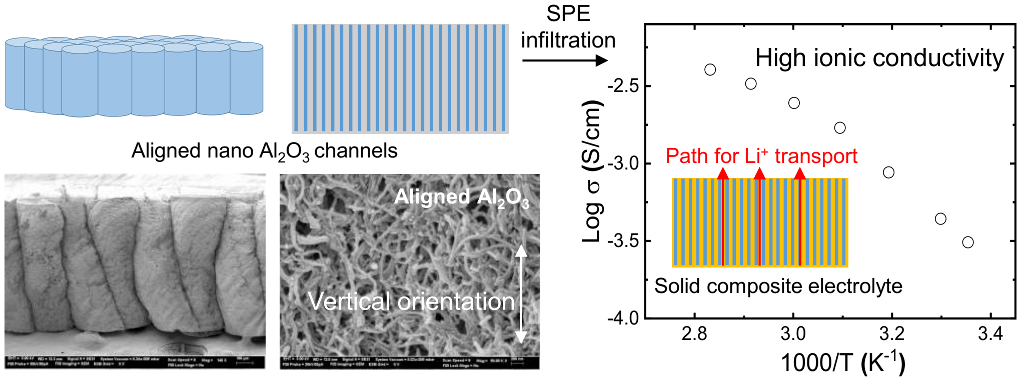


3D nano-architected structures for structural and functional applicatio

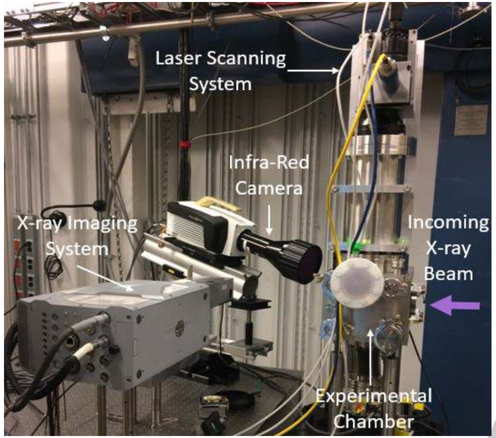
Application 1: Nano/macro-tunable architecture for structural application



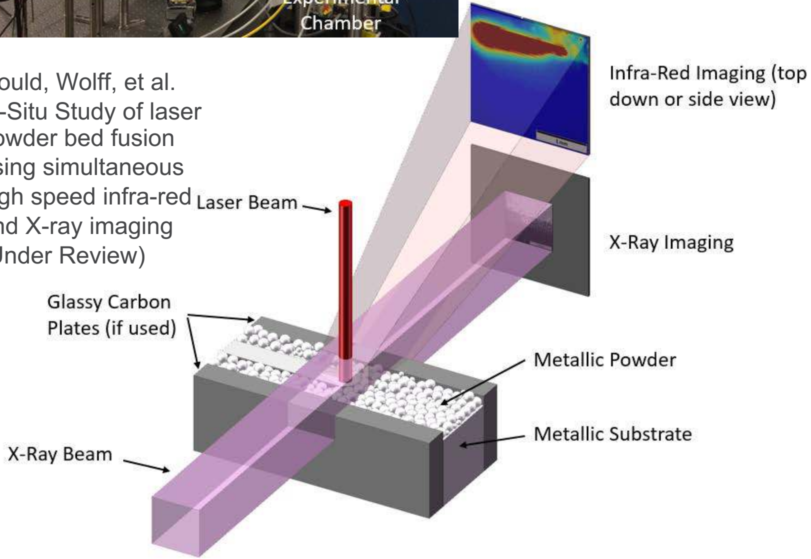
Application 2: Low-tortuosity architecture for energy application

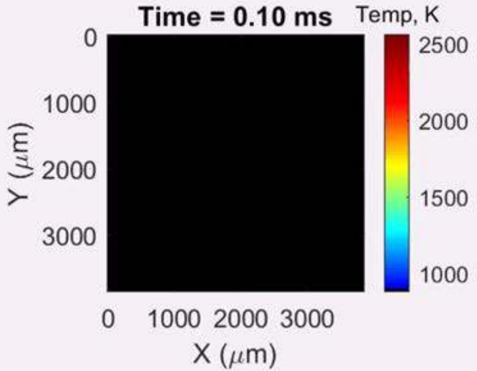


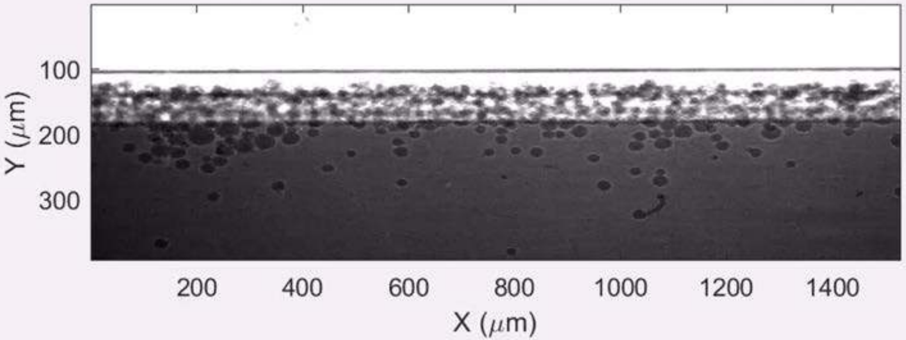
IN-SITU STUDIES OF MATERIAL SYNTHESIS AND PERFORMANCE



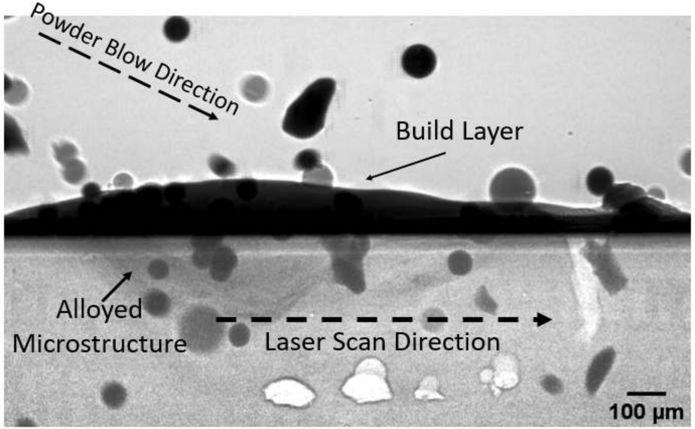
Gould, Wolff, et al.
In-Situ Study of laser powder bed fusion using simultaneous high speed infra-red and X-ray imaging
(Under Review)

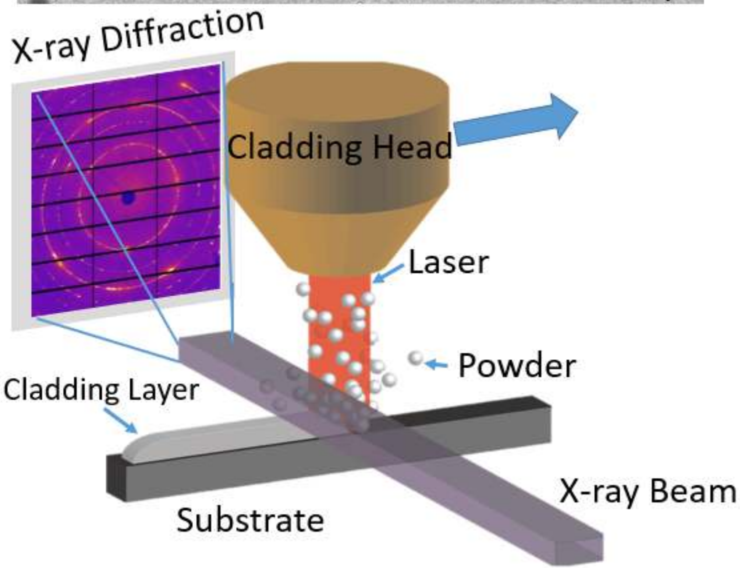


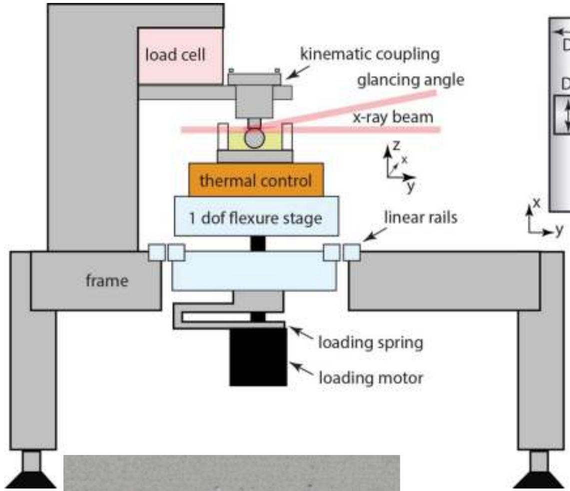


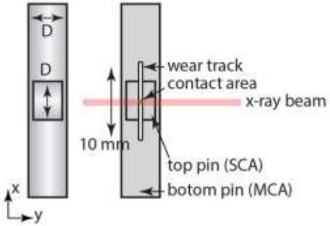


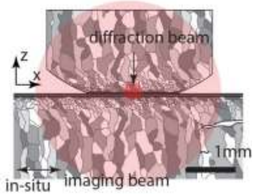
IN-SITU STUDIES OF MATERIAL SYNTHESIS AND PERFORMANCE

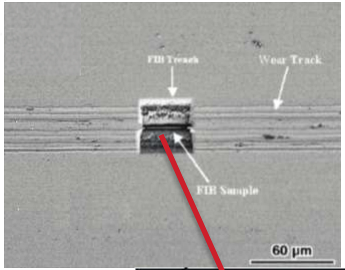


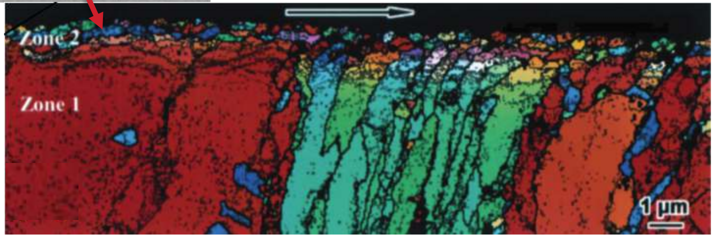






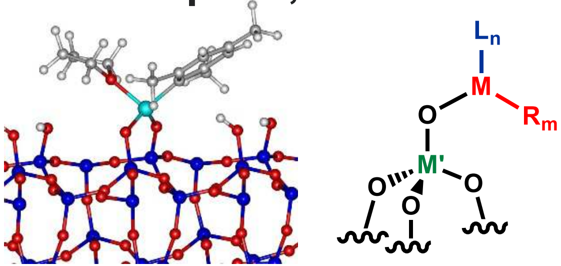






Catalysis Group at Argonne National Laboratory

David Kaphan, Chemical Science and Engineering, Argonne National Laboratory



Kaphan and co-workers *ACS Catal.* **2019**, ASAP
doi: 10.1021/acscatal.9b02800

Delferro and co-workers *Nat. Catal.* **2018**, *1*, 356 – 362.

Catalysis at ANL

Catalysis with Metal Organic Frameworks

Surface Organometallic Catalysis

Chemical Upcycling of Polymer Waste

Delferro and Coworkers, *ACS Cent. Sci.* **2019**, ASAP, doi: 10.1021/acscentsci.9b00722

Catalysis Group at Argonne National Laboratory

Homogenous

Well-defined precatalyst

Chemical tunability

Simple mechanistic analysis

Unstable coordination geometries

Surface Organometallic Chemistry

Easy synthesis

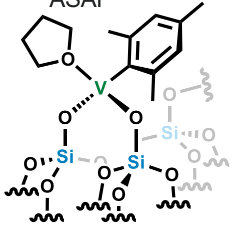
Facile separation

Thermally stable

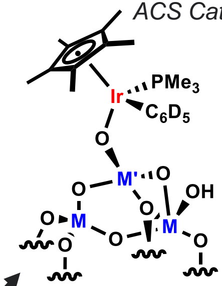
Site Isolation

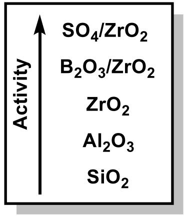
Heterogeneous

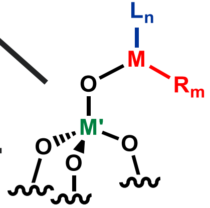
Mechanistic Aspects of a Surface Organovanadium(III) Catalyst for Hydrocarbon Hydrogenation and Dehydrogenation *Chem. Commun.* **2017**, *53*, 7325; *ACS Catal.* **2019**, ASAP



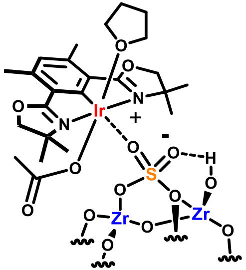
Surface Organometallic Chemistry of Supported Ir(III) as a Probe for Organotransition Metal−Support Interactions in C−H Activation *J. Am. Chem. Soc.* **2018**, *140*, 6308; *ACS Catal.* **2018**, *8*, 10058



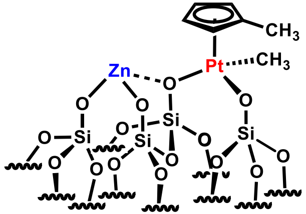




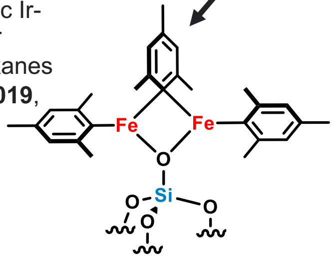
Surface Organometallic Chemistry



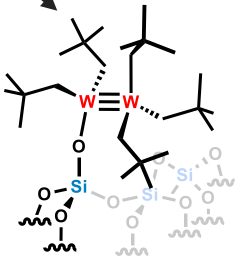
Supported Electrophilic Ir-Pincer Catalyst for Dehydrogenation of alkanes *J. Am. Chem. Soc.* **2019**, 141, 6325



Chemoselective Hydrogenation with Supported Organoplatinum(IV) Catalyst on Zn(II)-Modified Silica *J. Am. Chem. Soc.* **2018**, *140*, 3940 and *ACS Catal.* **2018**, *8*, 10058-10063



Nuclearity Effects in Supported, Single-Site Fe(II) Hydrogenation Catalysts *Dalton Trans.* **2018**, *47*, 10842



Supported Organo-Mo(III) and W(III) Dimer Catalysts for Olefins Metathesis

2019 UD-ANL WORKSHOP

NOVEMBER 21, 2019

UNIVERSITY OF DELAWARE

Argonne NATIONAL LABORATORY