U.S. ARMY COMBAT CAPABILITIES DEVELOPMENT COMMAND – ARMY RESEARCH LABORATORY

Development of a Methodology for High Throughput Materials Discovery for Protection Materials Under Extreme Loading Conditions

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Srikanth Singamaneni (WU St Louis)

Sinan Keten, Heather White, Wei Chen (NU)

Jhaoxu Meng (Clemson U)

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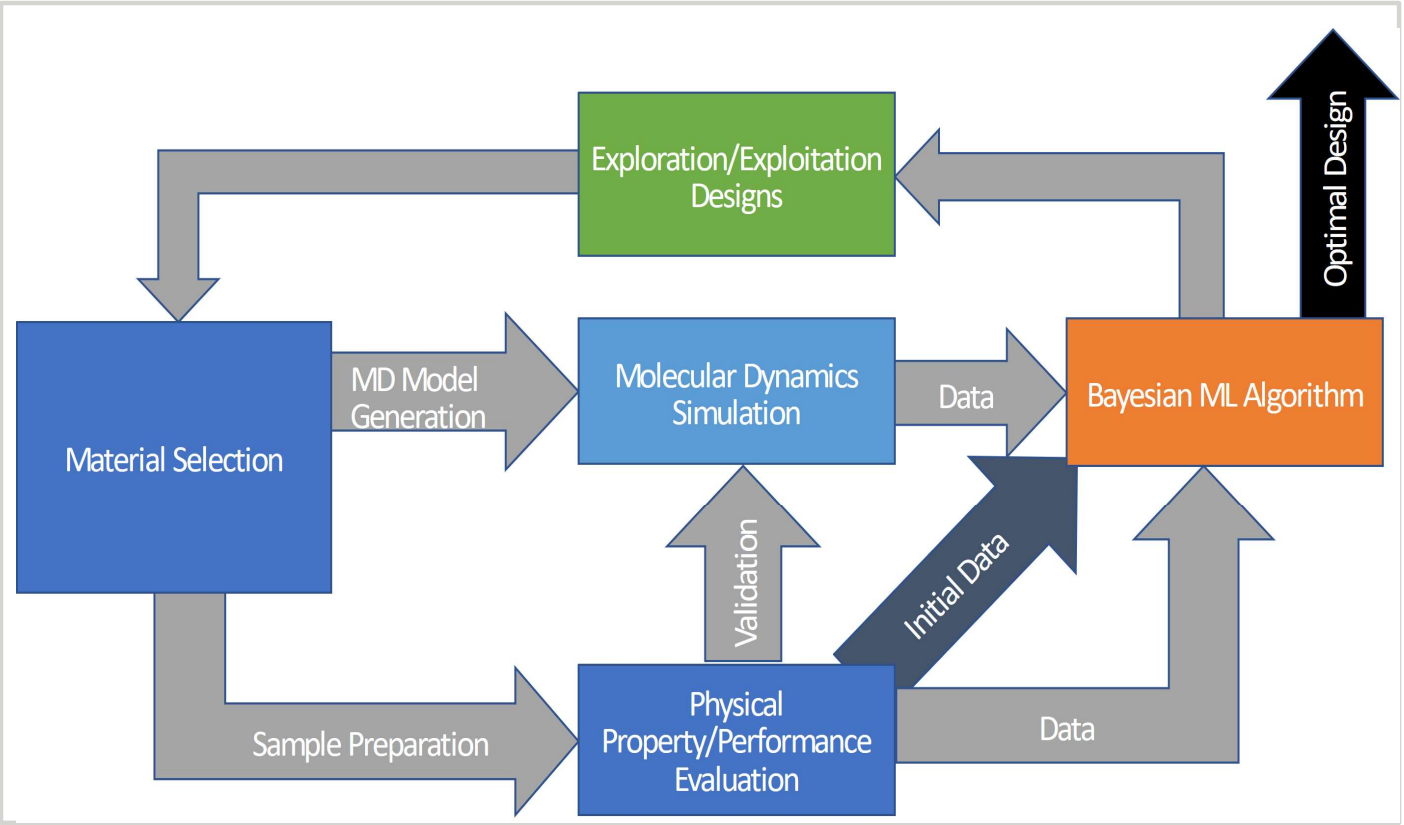
DEVELOPMENT OF A METHODOLOGY FOR HIGH THROUGHPUT MATERIALS DISCOVERY FOR PROTECTION MATERIALS UNDER EXTREME LOADING CONDITIONS

General Thrust Area: Data-driven Material Design



Accelerated discovery path to develop ballistic protection materials for drastically improved performance

Approach will link process-nano/micro structure-properties-performance

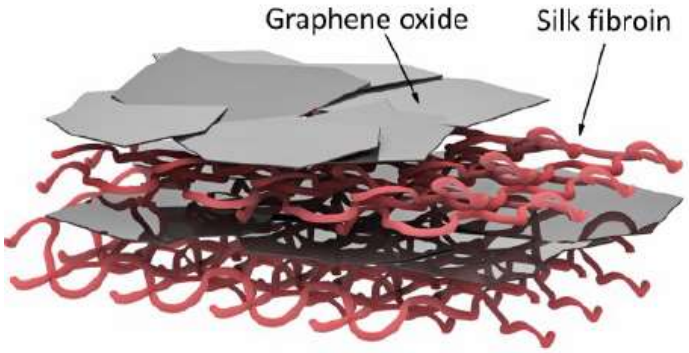
Initial materials: Graphene based nanocomposites

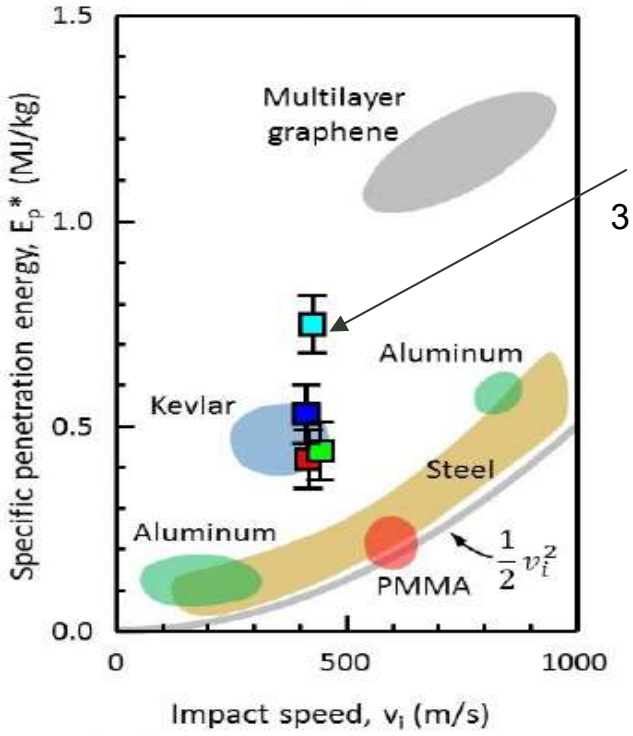
Develop and demonstrate a methodology that incorporates input from coarse grained MD simulations and data from material performance characterization experiments into a ML algorithm that would optimize the design of protection materials.

- Minimized number of experiments/simulations, minimized trial & error in design,
- Performance assessment criteria directly linked to ballistic performance: V50, Specific penetration energy, hole size, etc.

FIRST YEAR'S SCOPE :

- Experimental and Computational work on:
  - GO-silk fibroin composites
  - MLG-PC composites
- Implementation/adaptation of ML algorithm
- Assessment/validation of process flow





NANO LETTERS Letter
Cite This: Nano Lett. XXXX, XXX, XXX−XXX
pubs.acs.org/NanoLett

Extreme Mechanical Behavior of Nacre-Mimetic Graphene-Oxide and Silk Nanocomposites

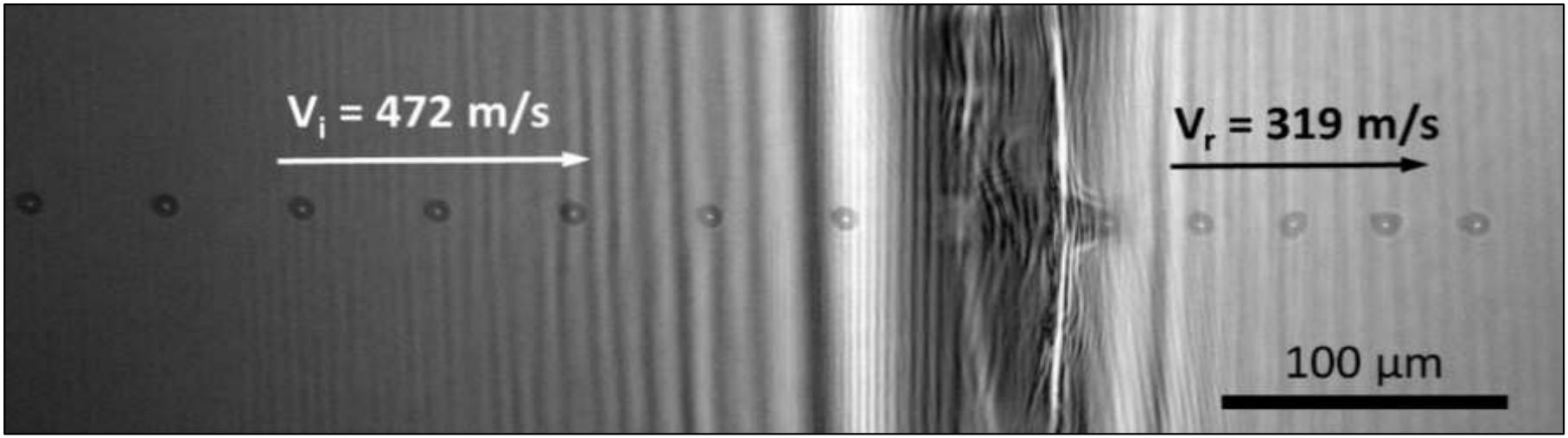
Wanting Xie,[†,‡] Sirimuvva Tadepalli,[§] Sang Hyun Park,[§] Amir Kazemi-Moridani,[‡] Qisheng Jiang,[§] Srikanth Singamaneni,[*,§] and Jae-Hwang Lee[*,‡]

PROPERTY/PERFORMANCE EVALUATION

Microballistics via laser-induced projectile impact test (LIPIT)

10^9 times reduction of the ballistic interaction volume

→ Extremely simplified mechanical characterization under extreme conditions



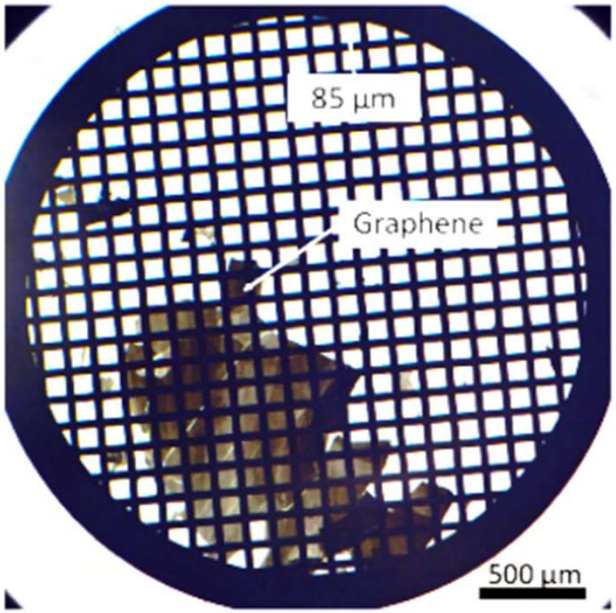
Source: Jae-Hwang Lee

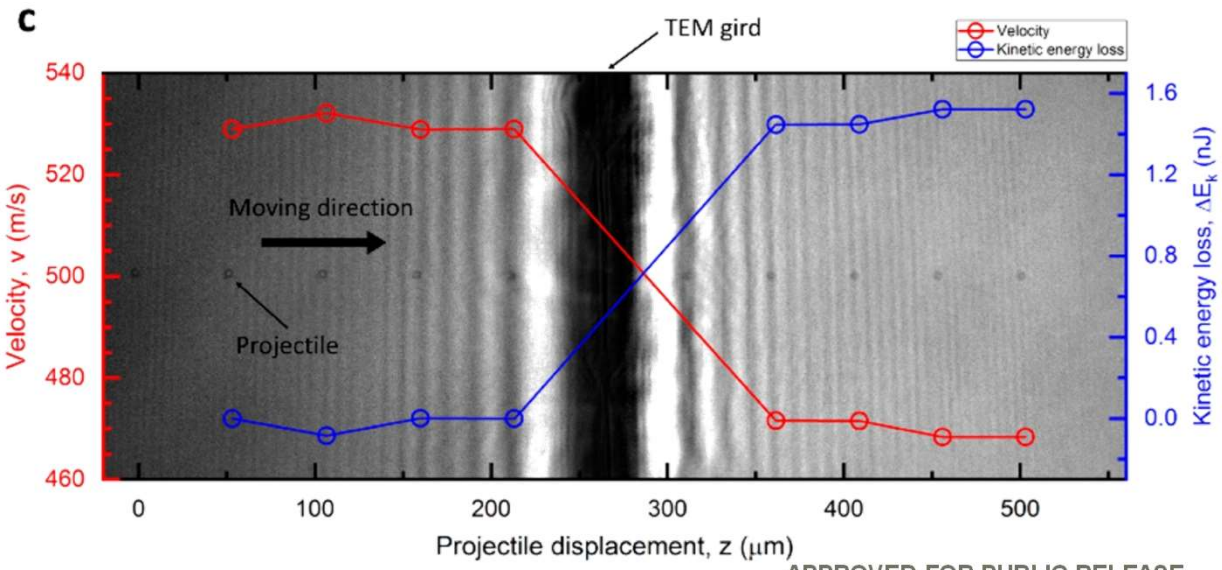
+ AFM, SEM, …

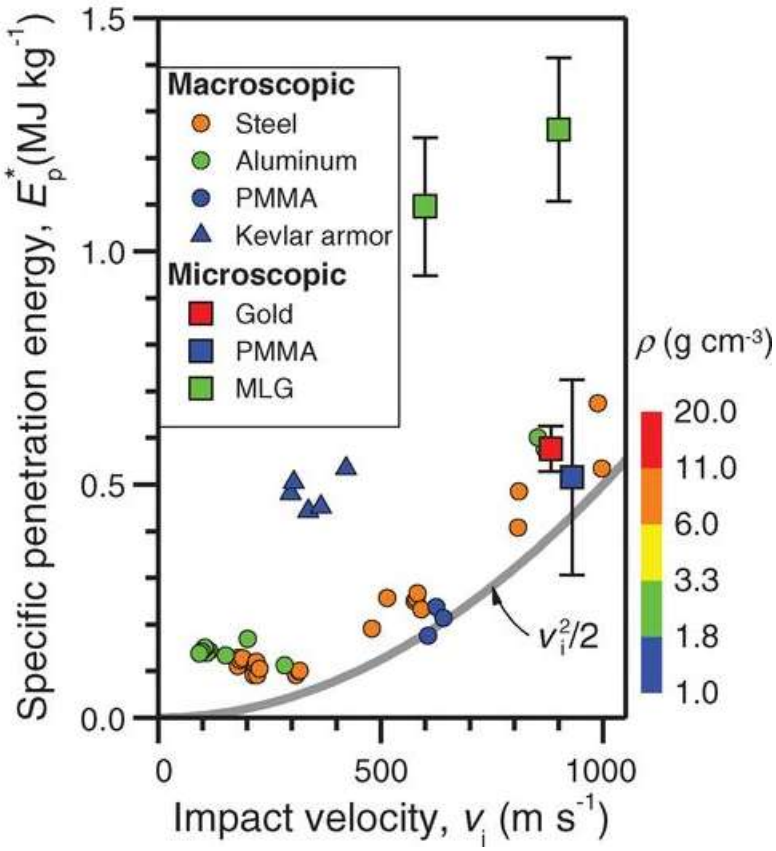
SPECIFIC PENETRATION ENERGY OF MLG

MLG demonstrates high E_p^* via its delocalization dynamics due to high speed of sound (>20 km/s)

$$E_{\mathrm{p}}^{*} \cong \frac{1}{2} v_{\mathrm{i}}^{2} + \frac{E_d}{(\rho h) A_{\mathrm{s}}}$$







Lee, J.-H. *et al.* Dynamic mechanical behavior of multilayer graphene via supersonic projectile penetration. *Science* **346**, 1092-1096 (2014). https://doi.org/10.1126/science.1258544

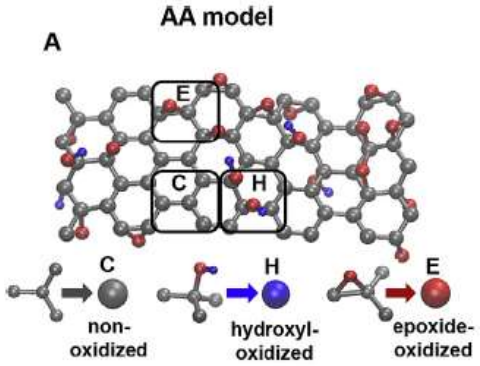
PRELIMINARY WORK ON GO STRUCTURE VARIATIONS

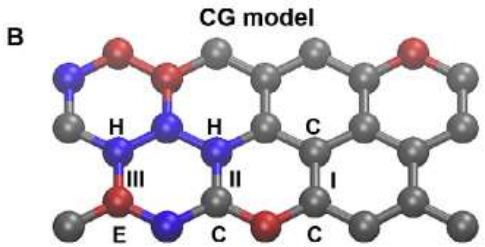
Manuscript in preparation

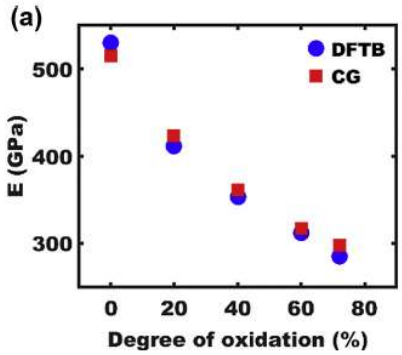
Contents removed.
Unpublished work.

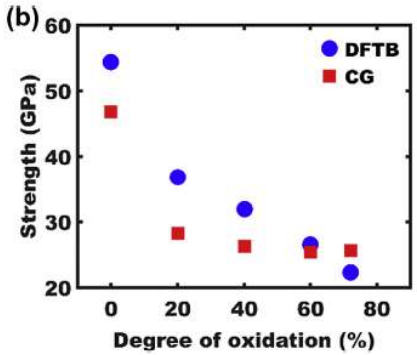
MULTILAYERED GRAPHENE OXIDE

- Leveraging pre-existing collaboration with Keten group (Northwestern University)
- Coarse-grained models for graphene oxide, graphene, polycarbonate, etc.
- Models implemented in LAMMPS, highly scalable for HTMDEC data needs
- MATLAB and Python scripts
- High-throughput computational data and modeling to inform the design process

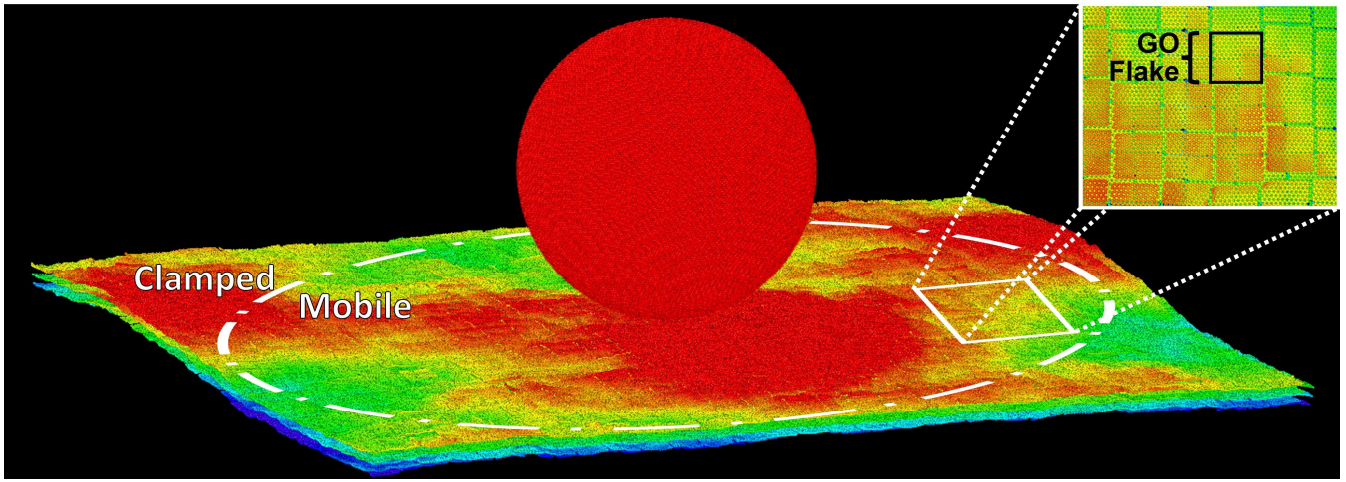






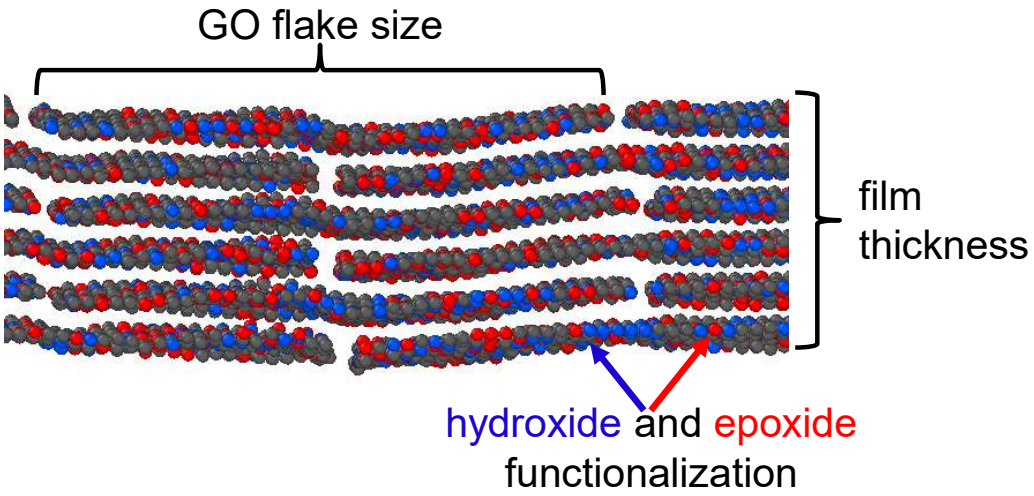


Molecular dynamics model for coarse-grained graphene oxide
(Meng, Soler-Crespo et al. 2017)

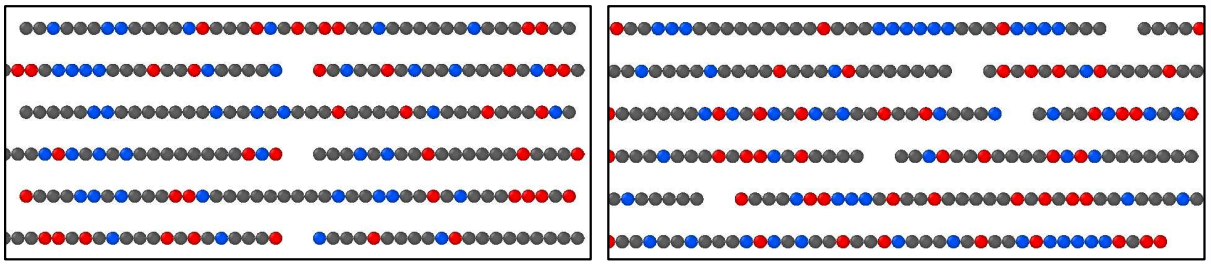


MULTILAYERED GRAPHENE OXIDE

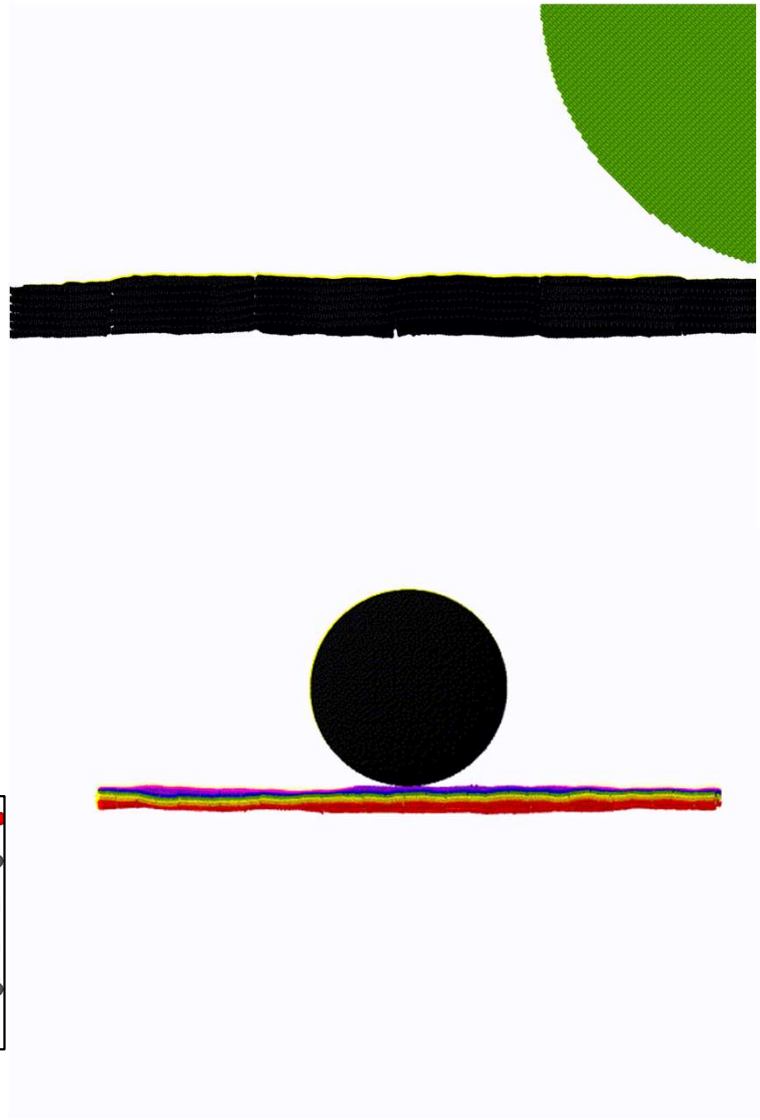
Molecular Design Variables



aligned vs random flake placement



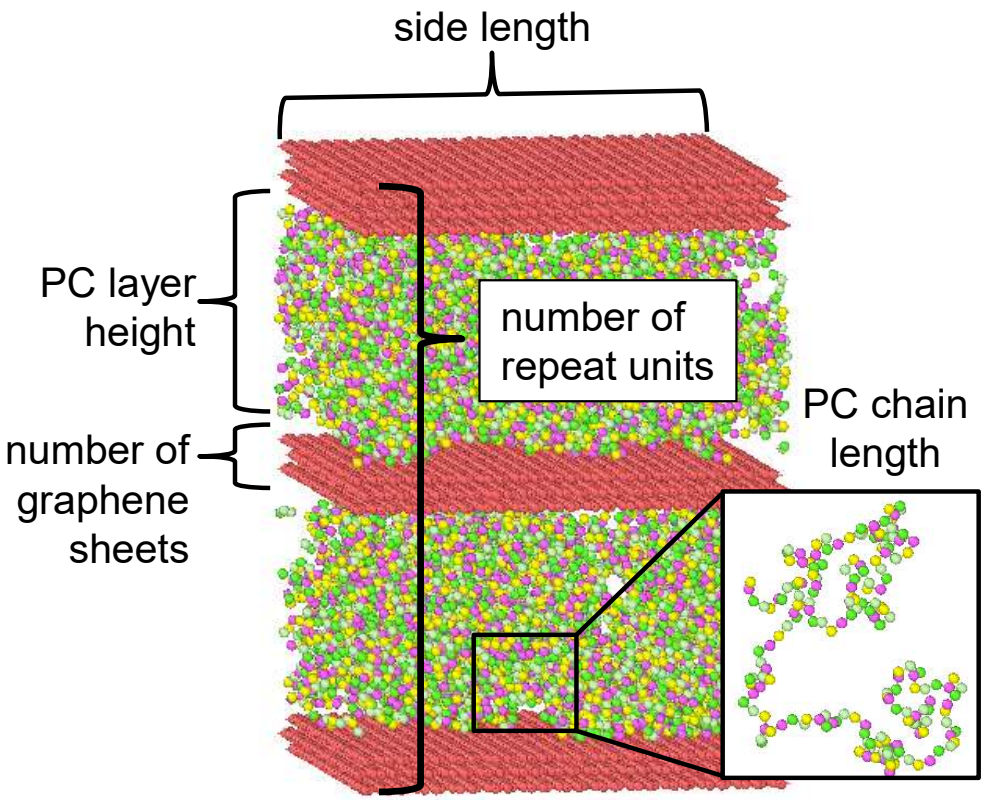
Simulation Results



White, Keten (NWU)

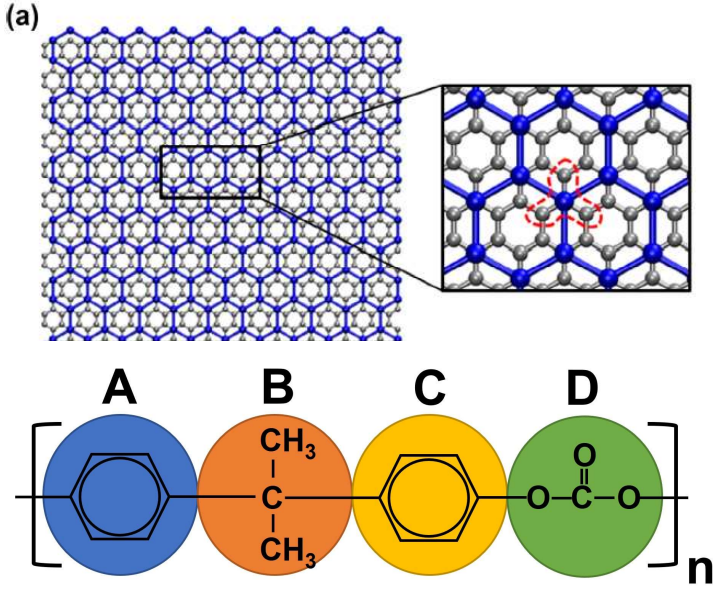
GRAPHENE / POLYCARBONATE COMPOSITES

Molecular Design Variables



- For graphene, same mapping from all-atom to coarse-grain as in MLGO systems (Ruiz, Xia et al. 2015)
- Coarse-grain model for PC and force field parameters from (Xia, Hansoge et al. 2019)

Coarse-grained Models



White, Keten (NWU)

GRAPHENE / POLYCARBONATE COMPOSITES

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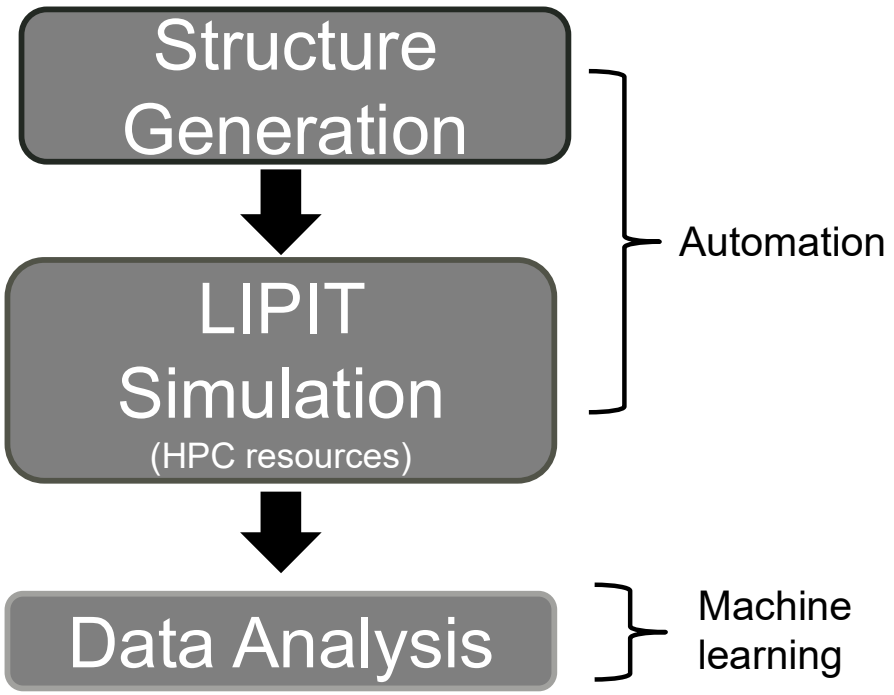
Unpublished work.

Automated workflow components

- Job scheduling
- Structure generation (Python script)
- Structure equilibration based on polymer chain statistics

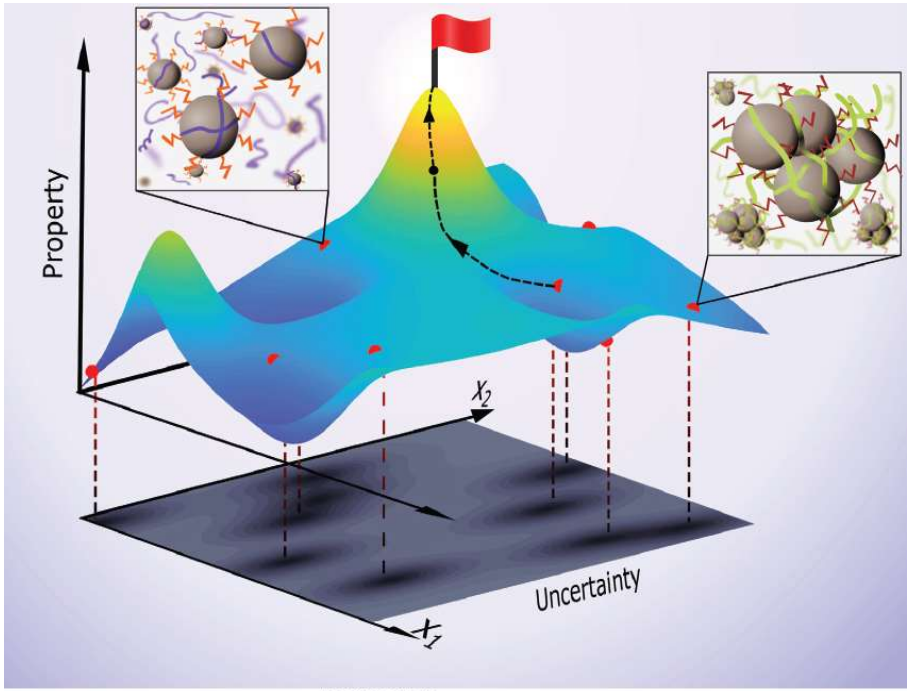


Coarse-grained molecular dynamics LIPIT simulations.
5 nm of PC with varying layers of graphene on each side.
Sliced views for clarity. [White, Keten (NU)]

Automated high-throughput simulations will provide a rich dataset to explore and model design space

MACHINE LEARNING --- LVGP BO

- latent variable Gaussian processes (developed by potential collaborator Wei Chen (NU)
  - Mixed variable ML
  - Uncertainty quantification



ISSN 2058-9689

ROYAL SOCIETY OF CHEMISTRY

PAPER
Wei Chen *et al.*
Data centric nanocomposites design *via* mixed-variable Bayesian optimization

IChemE

ACS NANO

Cite This: *ACS Nano* 2018, 12, 7946–7958 www.acsnano.org

ARTICLE

Materials by Design for Stiff and Tough Hairy Nanoparticle Assemblies

Nitin K. Hansoge,[†] Tianyu Huang,[†] Robert Sinko,[†,‡] Wenjie Xia,[*,§,∥] Wei Chen,[*,†,∥] and Sinan Keten[*,†,∥,⊥]

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Systematic coarse-graining of epoxy resins with machine learning-informed energy renormalization

Andrea Giuntoli[1,2], Nitin K. Hansoge[2,3], Anton van Beek[2,3], Zhaoxu Meng[4✉], Wei Chen[2,3✉] and Sinan Keten[1,2,3✉]

SCIENTIFIC REPORTS
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Bayesian Optimization for Materials Design with Mixed Quantitative and Qualitative Variables

Yichi Zhang[1], Daniel W. Apley[2] & Wei Chen[1*]

QUESTIONS

COMMENTS

COLLABORATION DISCUSSIONS

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