



Computational Design of Multifunctional Materials and Structures

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Integrated DDesign Automation Laboratory (*IDEAL*)

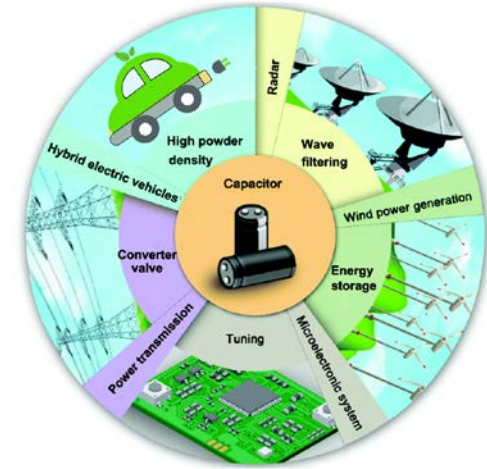
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IDEAL Lab: Design of Microstructural Material Systems

Design of composition, morphology, and synthesis methods of nanodielectrics

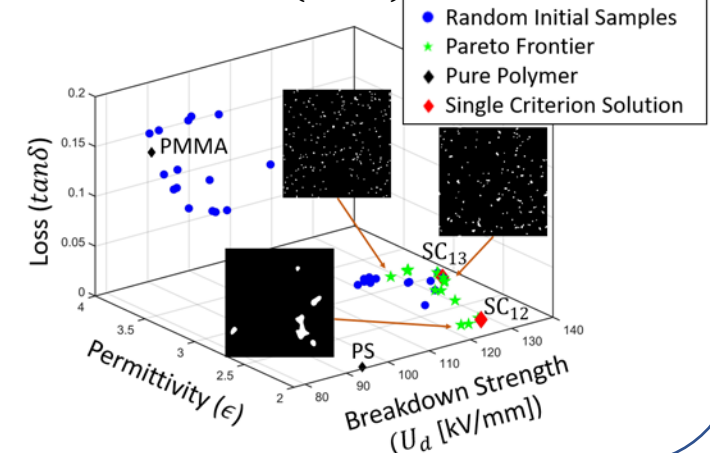


Multifunctional nanodielectrics

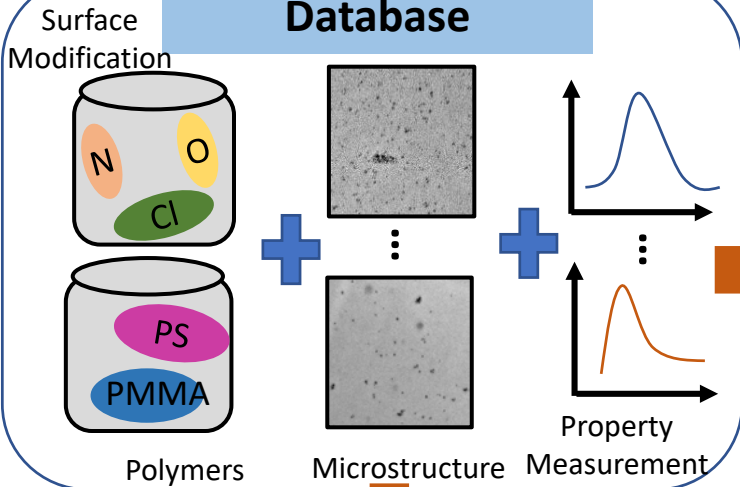
- Storage
- Insulation
- Endurance

5. Mixed-Variable Multicriteria Bayesian Optimization

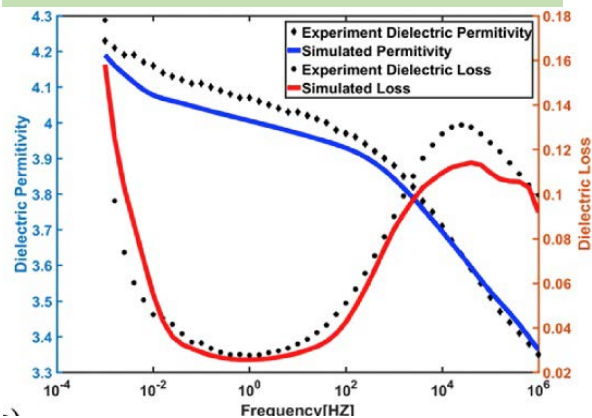
- maximize **Breakdown Strength** (U_d)
- minimize **Dielectric Permittivity** (ϵ)
- minimize **Dielectric Loss** ($\tan\delta$)



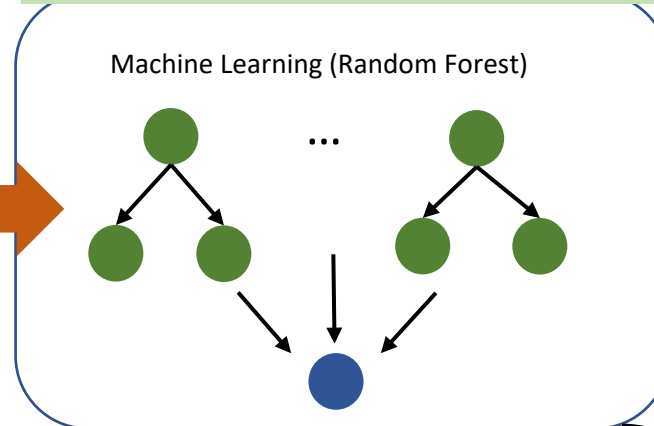
1. Nanocomposite Database



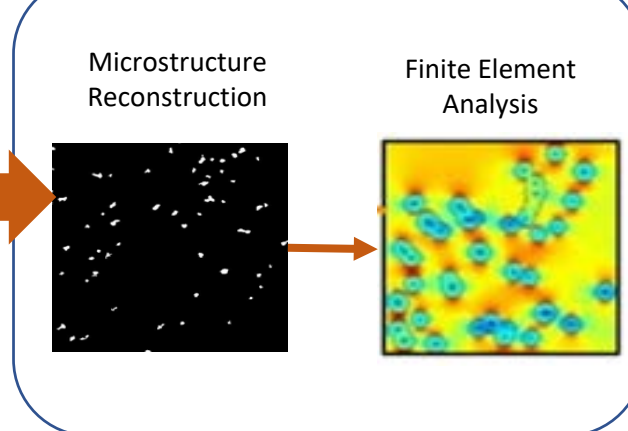
2. Interphase Calibration



4. Machine Learning for S-P Prediction



3. FEM based S-P Simulation



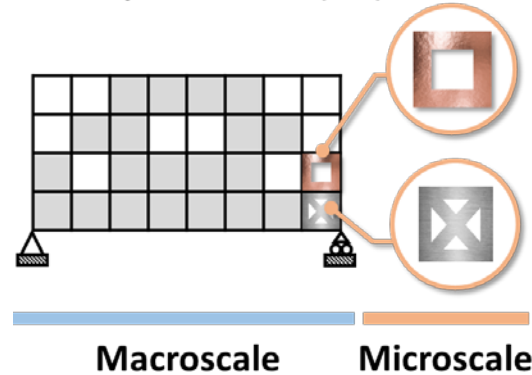
IDEAL Lab: Data-Driven Design of Heterogenous Material Systems

Multiscale design of constituent materials and architectures in light weight, deformable structures

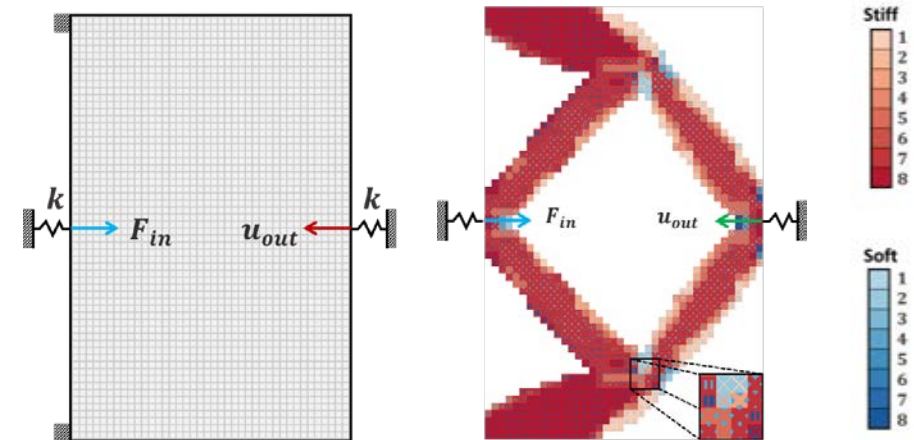
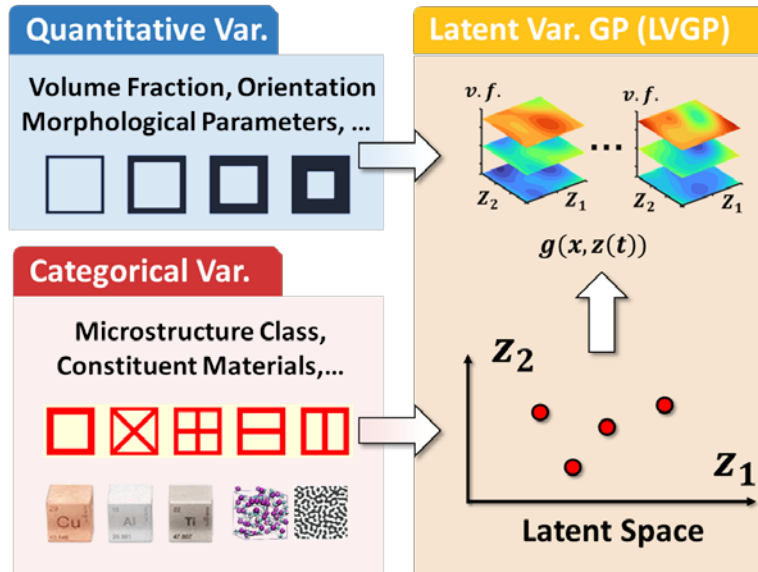
Unit Cell Properties

- Stiffness
- Thermal Conduction Coefficients
- ...

Multiscale Topology Optimization (TO)



Ion et al. UNIST, 2016



u_{out} +167% displacement than periodic design

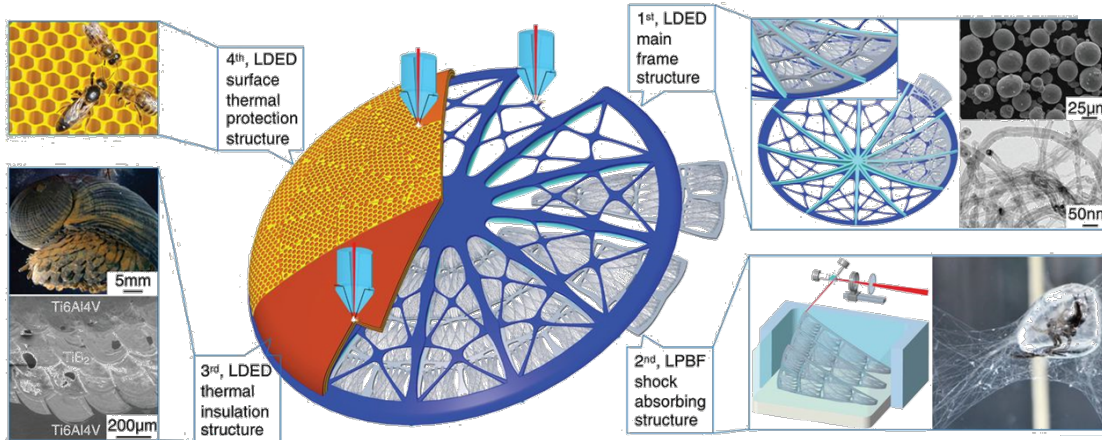
Multiclass Multi-Material Compliant Mechanism

Wang, L., Tao, S., Zhu, P., and Chen, W., ASME Journal of Mechanical Design, 2021

Challenging Computational Design of Multifunctional Systems

Heterogeneous Materials – Curse of Dimensionality

- Multiscale modeling & design/ material-structural design



Gu's group at Nanjing University of Aeronautics and Astronautics (Gu, D., et al. Science, 2021)

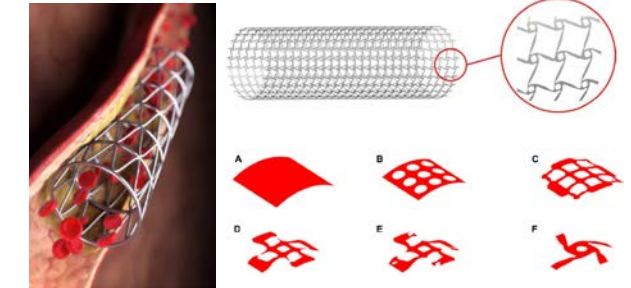
Nonlinear Behaviors

- Accuracy and cost tradeoff
- lack of analytical gradient for optimization



Energy Absorption

Valdevit & Rimoli groups
(Bauer, J., et al. 2021)

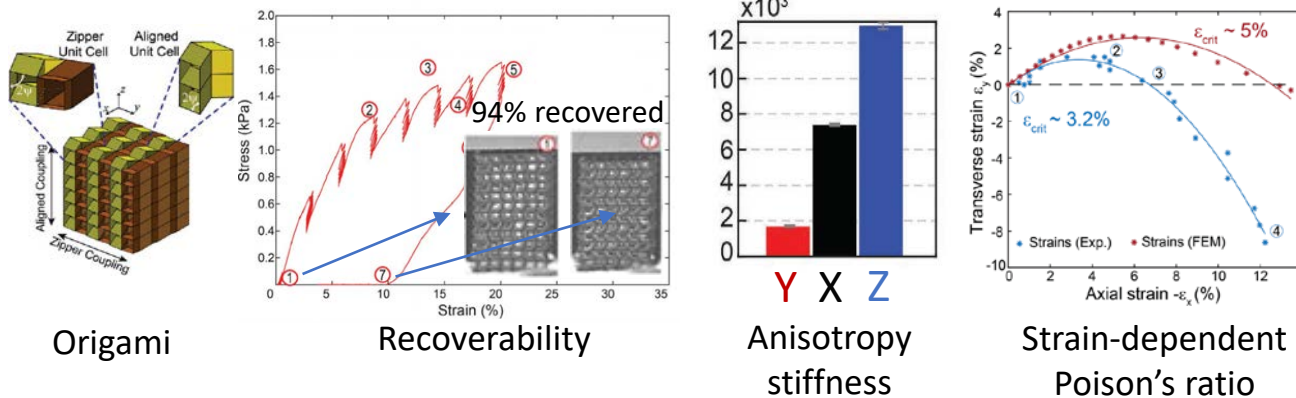


Coronary stent

Source | www.thecardiologyspecialist.com
Luo's group at University of Technology Sydney
(Xue, H., et al. 2020)

Multistable Systems

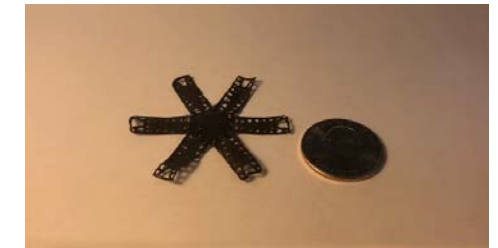
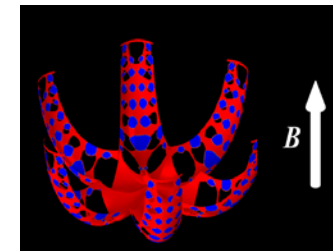
- Non-differentiable behavior



Paulino, Espinosa, & Krishnaswamy groups (Lin, Z., et al. 2020)

Multiphysics Active Metamaterials

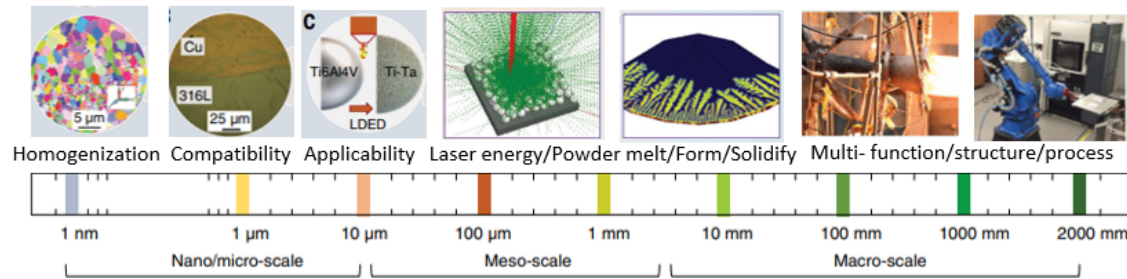
- Expanded design space of external stimulus
- Coupling effects



Chen's group at SUNY
(Tian et al 2021)

Convergence Opportunities: Integrating Materials, Mechanics, Manufacturing and Design

Predicting process-structure-property-performance-function relation across multiple scales with UQ



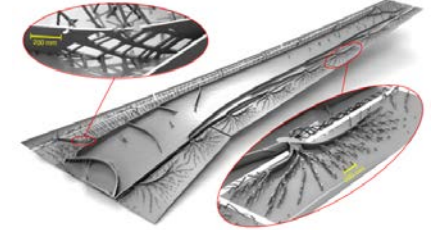
Gu's group at Nanjing University of Aeronautics and Astronautics (Gu et al. 2021)

Supercomputing and AI techniques for fast 3D design integration and exploration



Lightweight Bridge Design
($>10^6$ elements)

source | Kim's group at USCD
(<http://m2do.ucsd.edu/research/?topic=mdao>)

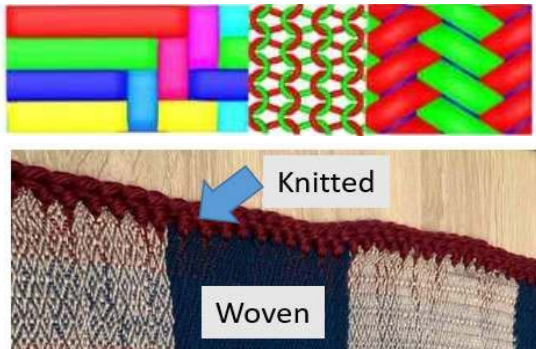


"Giga-voxel" TO of Wing
($>10^9$ elements)

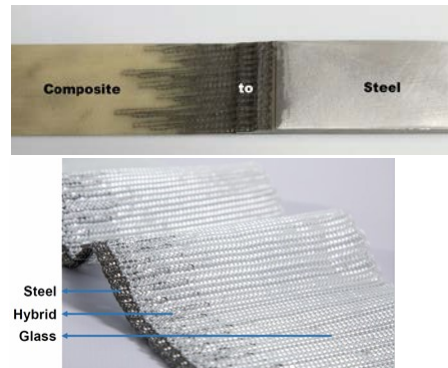
Sigmund's group at DTU
(Aage et al. 2017)

Multiscale design framework for heterogeneous systems to exploit hybrid manufacturing capability

- Hybrid manufacturing



Cao's group at Northwestern

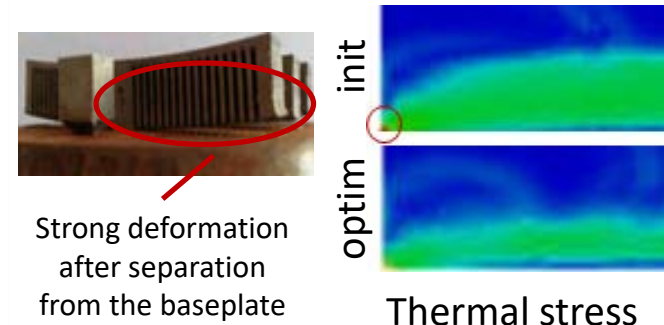


Knitted Composite Steel Joint

Gardiner, G. Composites World, 2019
source | Hyconnect, FAUSST Joint

Integrating manufacturing process impact into topology optimization

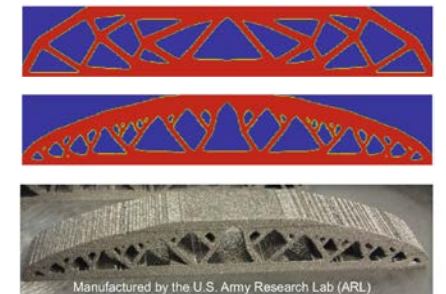
- Reducing residual stress
- Overhang-free design



Strong deformation
after separation
from the baseplate

Thermal stress

Allaire's group at Ecole Polytechnique, France
(Allaire et al. 2018)



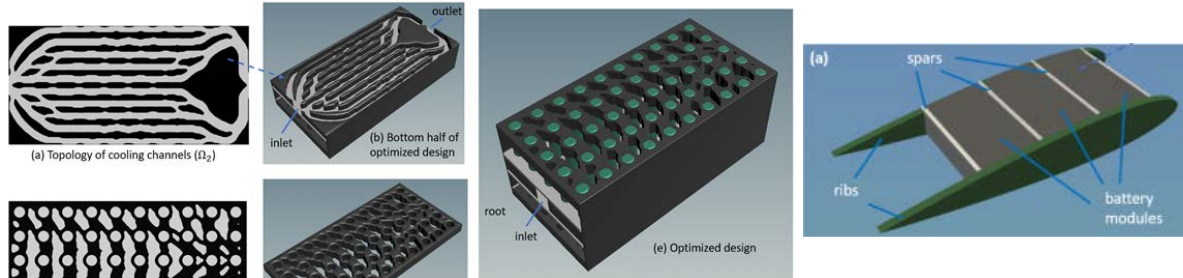
Optimized MBB Beam

Guest's group at JHU
(Gaynor & Guest 2016)

Chen Backup Slides

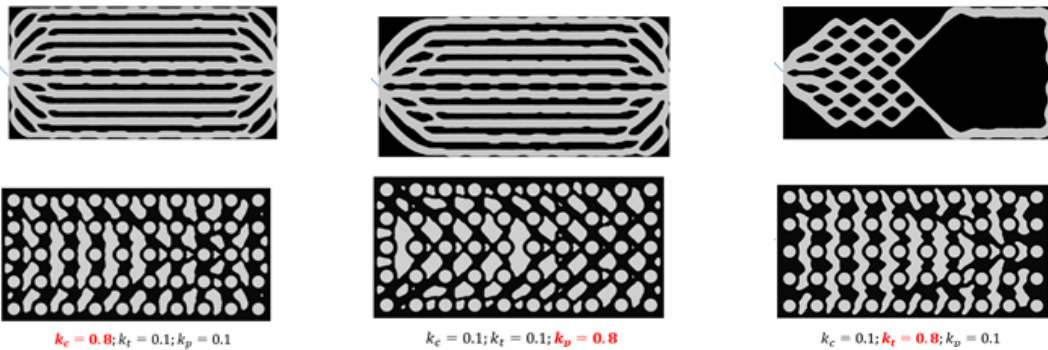
Existing Multiphysics & Multifunctional Topology Optimization

- Level set TO method for load carrying battery packs (fluid-thermal-mechanics)



Battery modules placed between adjacent ribs and spars.

Equal weighted for all physics



High weights on **mechanical**
(strain energy)

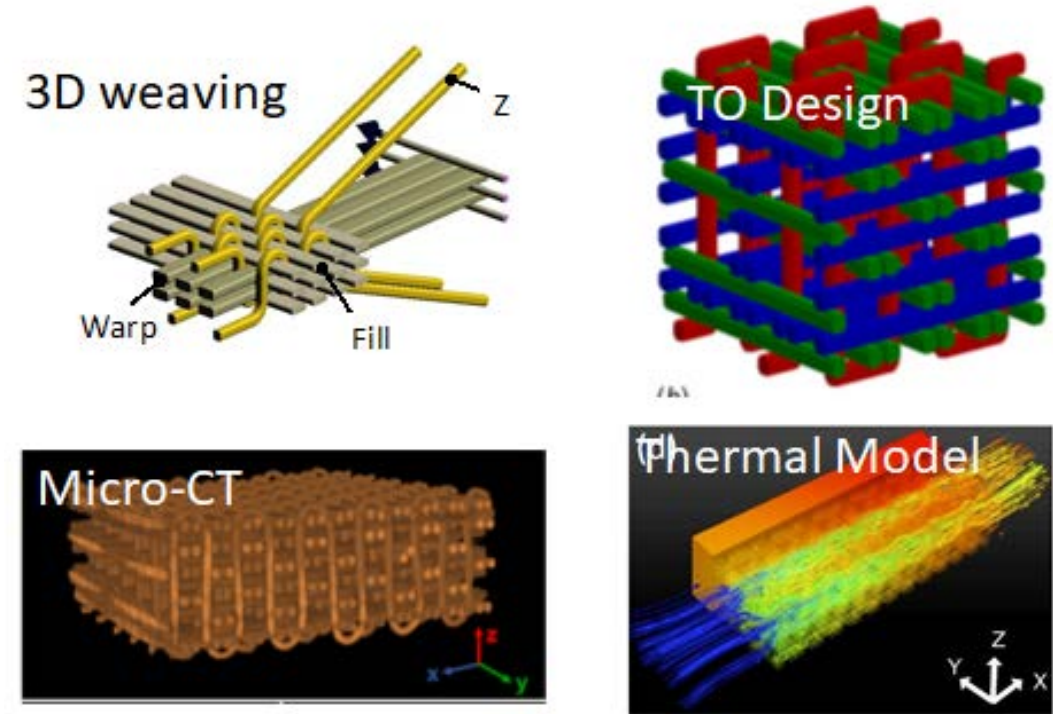
on **fluid** (flow
pressure diff.)

on **thermal** (ave.
temp.)

Kim's group at UCSD (Kambampati et al. 2021)

- Ground structure representation of 3D woven metallic lattices (max permeability)

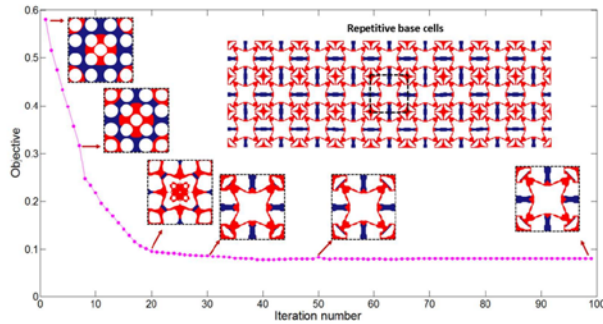
Manufacturable lattices with enhanced fluidic and thermal properties for heat transfer applications.



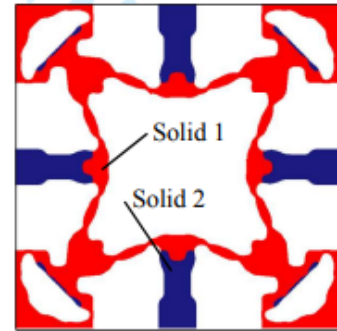
*Guest's group at JHU
(Zhao et al 2015; Zhao et al 2017; Ha et al 2019)*

Existing Multimaterial & Multifunctional Topology Optimization

- Negative Poisson's Ratio (NPR) & Negative Thermal Expansion (NTE)

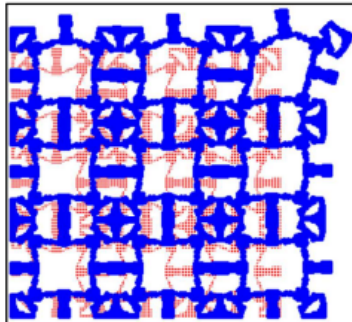


Multi-objective topology optimization

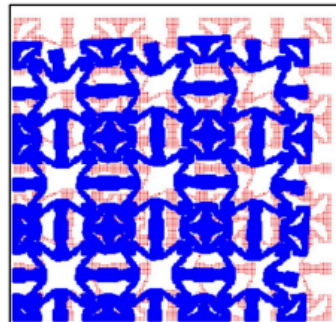


Optimized Topology

Simultaneous realization of NPR and NTE that are difficult to achieve with only one constitutive material



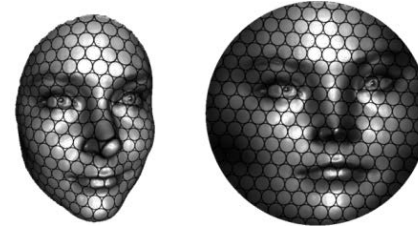
Deformation 1 (elastic)



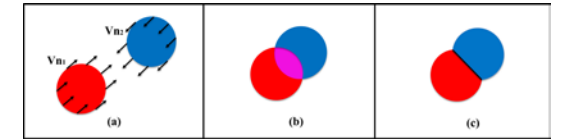
Deformation 2 (thermal)

Luo's group at University of Technology, Sydney (Wang et al 2017)

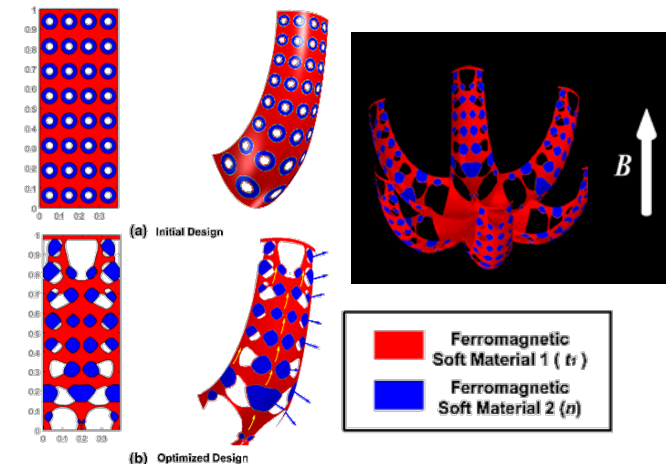
- Conformal design of active ferromagnetic system



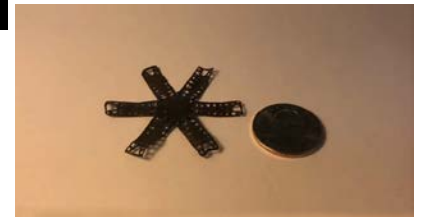
Conformal mapping (3D -> 2D)



Reconciled level set method



Optimized multi-material flytrap shell actuator



Chen's group at SUNY
(Tian et al 2021)