From Quantum Mechanics to Battery Design: Uncovering the Materials World with Computation
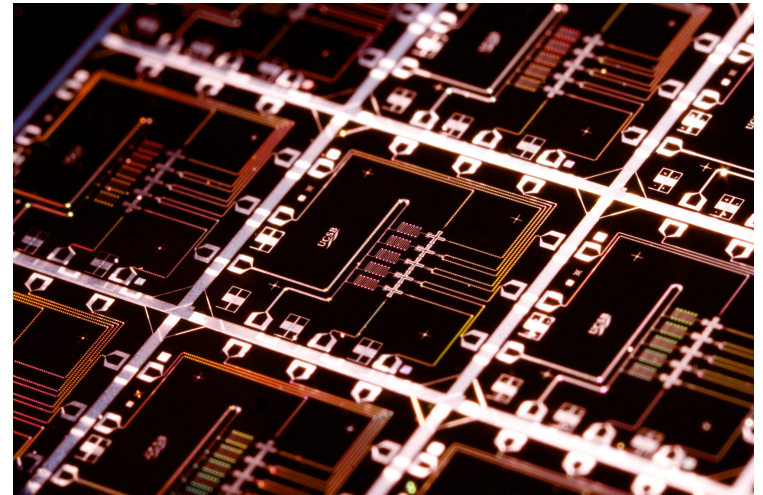
Nima Leclerc
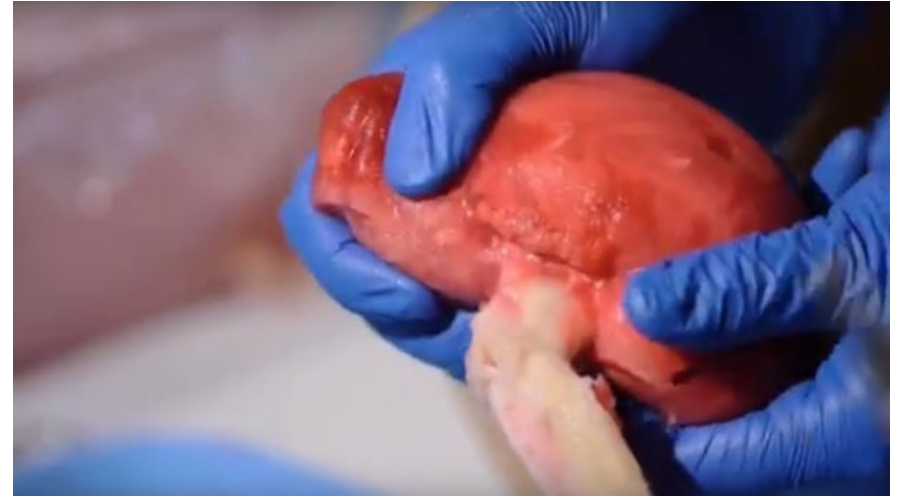
Jena-Xing Group

Department of Materials Science and Engineering
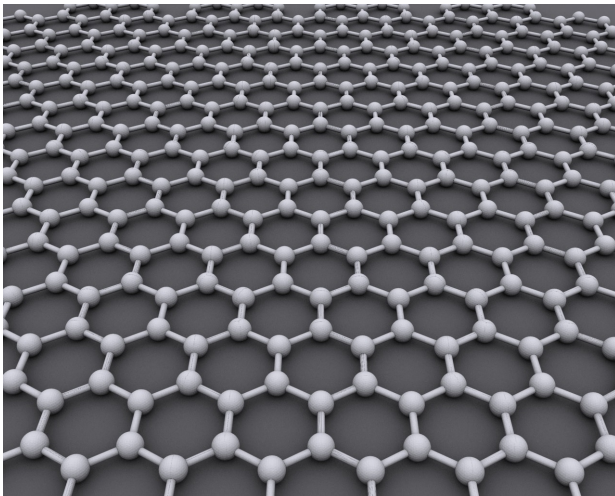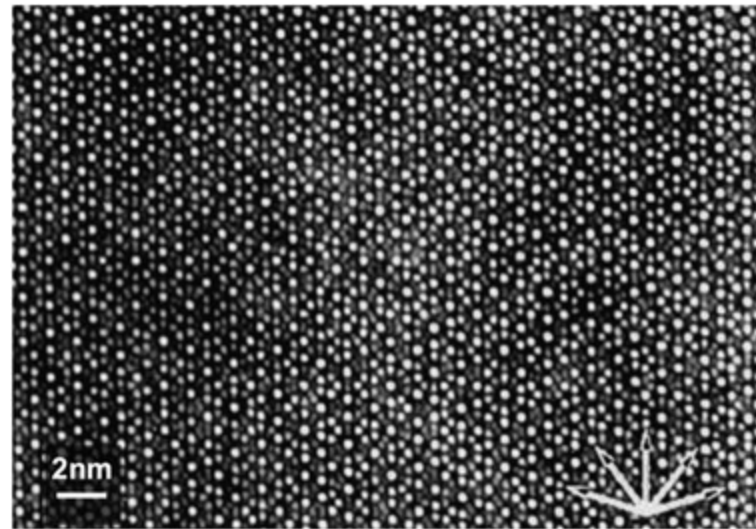
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Why care about materials?

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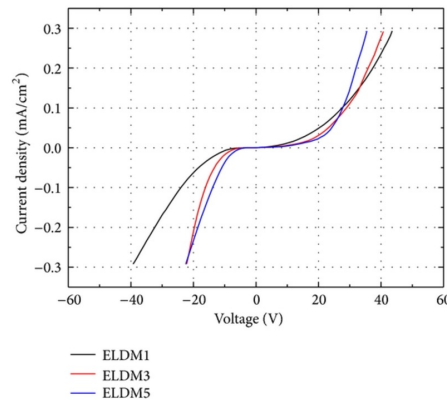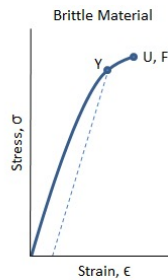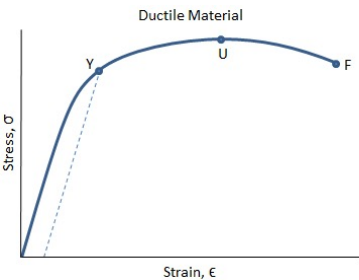# Making materials= Problem ??

2nm

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Solution=Physics + Computation
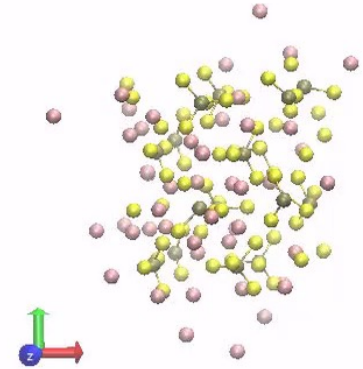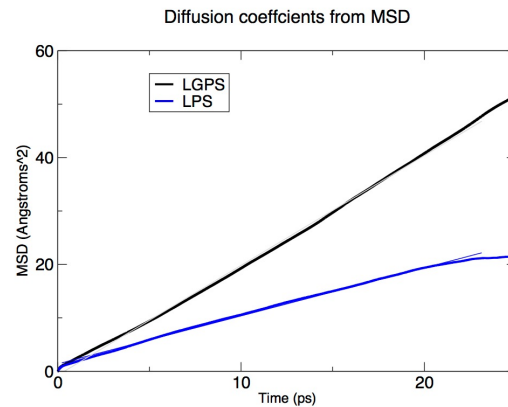
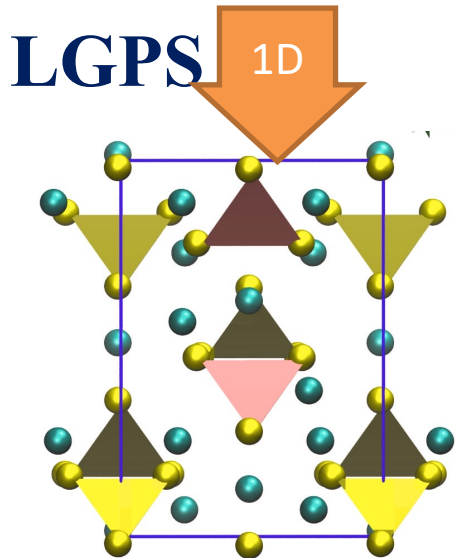$$[-\nabla^2 + \hat{V}]|\Psi\rangle = \epsilon|\Psi\rangle$$

$$\hat{H}|\Psi\rangle = [-\frac{\bar{h}^2}{2m_e}\sum_i \nabla_i^2 - \sum_{i,I}\frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} - \frac{\bar{h}^2}{2M_I}\sum_I \nabla_I^2 + \frac{1}{2}\sum_{I\neq J}\frac{e^2}{|\mathbf{r}_I - \mathbf{R}_J|}]|\Psi\rangle = \epsilon|\Psi\rangle$$
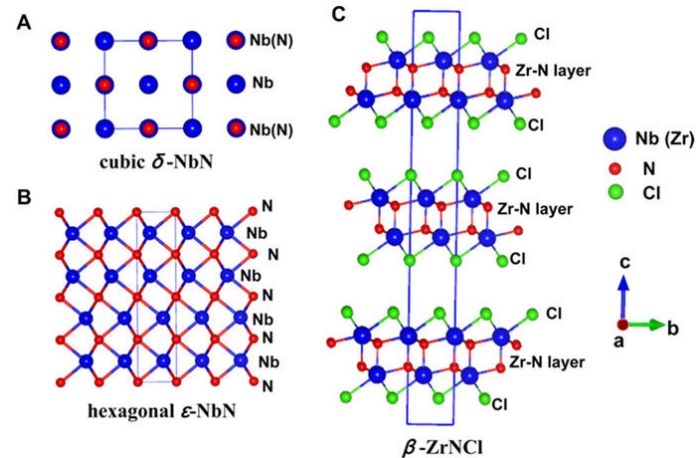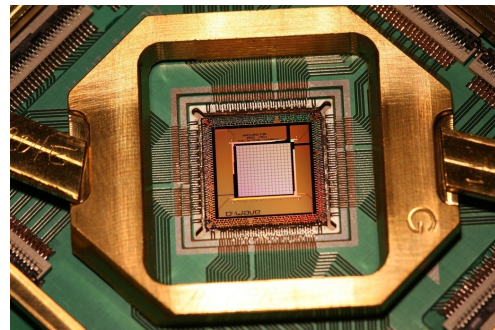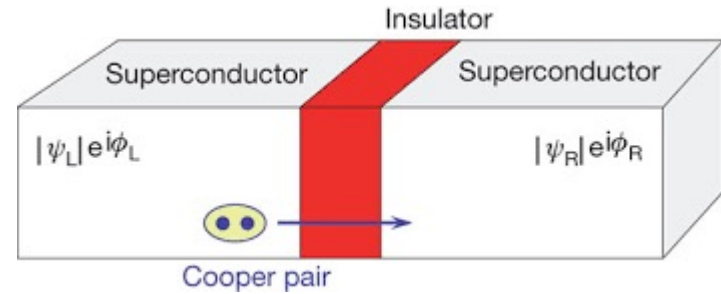
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Solving the Energy Crisis with a Computer?

LGPS 1D

Diffusion coeffcients from MSD

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Quantum Computing with Quantum and Computers

Insulator

Superconductor | Superconductor

$|\psi_L|e^{i\phi_L}$ | $|\psi_R|e^{i\phi_R}$

Cooper pair

A

cubic δ-NbN

Nb(N)
Nb
Nb(N)

B

hexagonal ε-NbN

N
Nb
N
Nb
N
Nb
N
Nb
N

C

Cl
Zr-N layer
Cl

Nb (Zr)
N
Cl

Cl
Zr-N layer
Cl

Cl
Zr-N layer
Cl

β-ZrNCl

c
a   b

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Yay Innovation!!

Thank you collaborators and funding agencies.

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