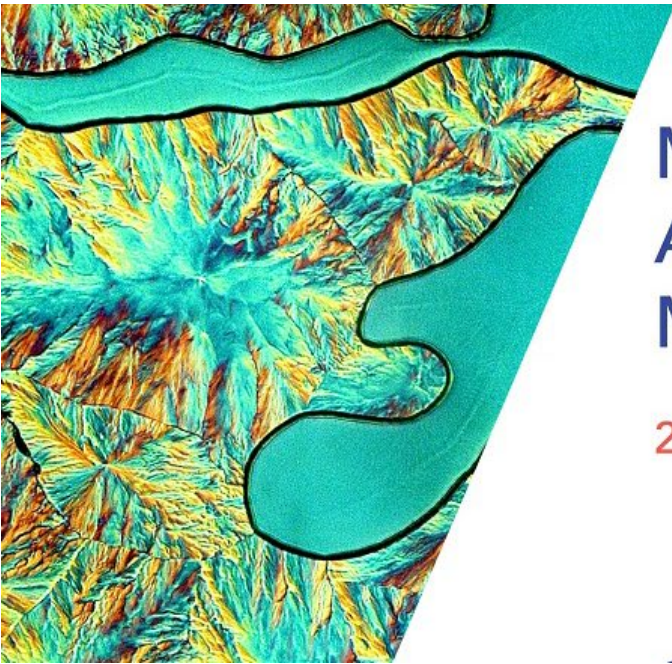


# Machine Learning for Accelerated and Inverse Metasurface Design

Presented by:



# The OSA Photonic Metamaterials Technical Group Welcomes You!



## MACHINE LEARNING FOR ACCELERATED AND INVERSE METASURFACE DESIGN

2 April 2020 • 13:00 EDT



Photonic  
Metamaterials  
Technical Group

# Technical Group Leadership 2020

Chair



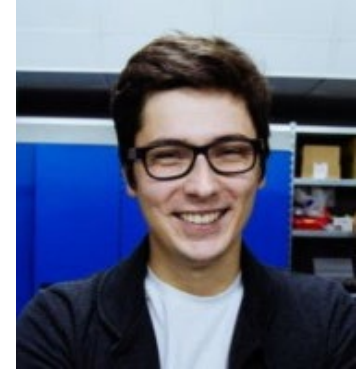
**Wei Ting Chen**  
Harvard Univ.

Webinar Officer



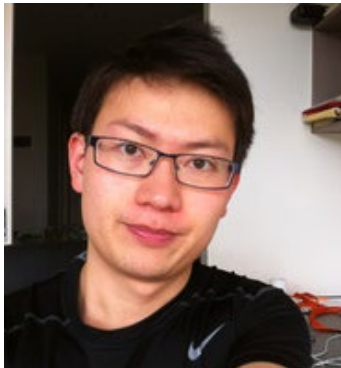
**Aaron Joseph Pung**  
Sandia National Laboratories

Webinar Officer



**Maxim Shcherbakov**  
Cornell Univ.

Event Officer



**Haoran Ren**  
LMU Munich

Event Officer



**Md Saad-Bin-Alam**  
University of Ottawa



Photonic  
Metamaterials  
Technical Group

# Technical Group at a Glance

- Total Members: 1,516 members
  - A part of benefits of OSA membership
- Mission and Focus
  - Serve the community by sharing latest information and providing a pathway for young professionals to greater involvement with mentors and peers

- OSA Incubator on Flat Optics: Recent Advances and Future Opportunities



#OSAMetamaterialsTG

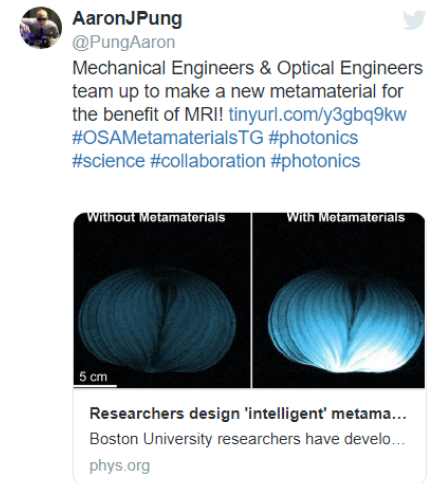
Join Our Online Community

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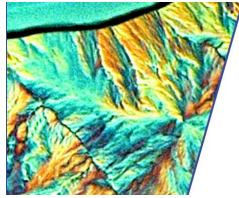
Curated Tweets by @hwwalter

Featured tweets from the OSA Photonic Metamaterials Technical Group



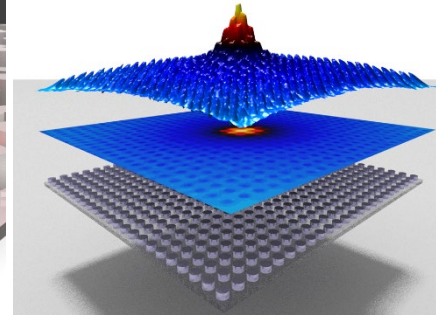
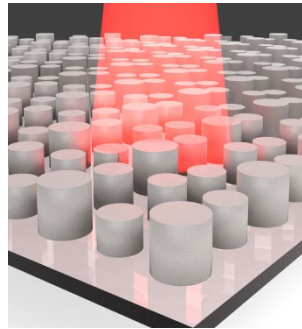
- Upcoming webinars from Prof. Federico Capasso (Harvard) and Prof. Andrea Alu (CUNY)





## Machine Learning for Accelerated and Inverse Metasurface Design

Thursday, April 2<sup>nd</sup>, 13:00 EDT



Speaker: Dr. Willie Padilla  
Full Professor in the Department of ECE at Duke University



# Machine Learning for Accelerated and Inverse Metasurface Design



WILLIE PADILLA

DUKE UNIVERSITY



# ACKNOWLEDGEMENTS

## Graduate Students

Christian Nadell (CoVar Applied Tech)  
Simiao Ren (Duke)  
Bohao Huang (Duke)

## Collaborators

Kebin Fan (Duke)  
Jordan Malof, (Duke)

## Funding



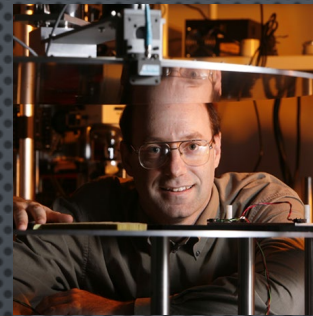
DE-SC0014372





# CENTER FOR METAMATERIALS AND INTEGRATED PLASMONICS DUKE UNIVERSITY

The screenshot shows the homepage of the Center for Metamaterials and Integrated Plasmonics (CMIP) at Duke University. The header includes the CMIP logo and navigation links: HOME, ABOUT, RESEARCH, PUBLICATIONS, NEWS, CONFERENCES, POSITIONS, CONTACT. The main content area features a large banner for 'KYMETA' with a video player and a 'MOST VIEWED' section. The 'TOPICS' section is divided into METAMATERIALS, PLASMONICS, and ACOUSTICS, with sub-sections for Retrieval, Communications, Origins, and A Definition. The 'NEWS' section includes articles like 'CMIP Seminar: Controlling waves in complex media: from time reversal to wave front shaping via metamaterials' and 'Meanwhile in the Future – Gizmodo Podcast'. A 'PHOTO GALLERY' is also visible at the bottom.



David Smith



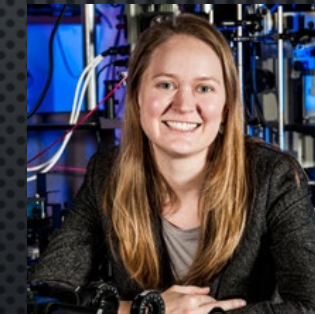
Nan Jokerst



Steve Cummer



Natalia Litchinitser



Maiken Mikkelsen

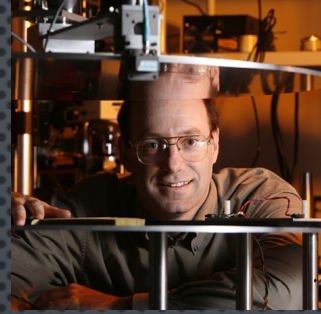


Willie Padilla

Non-linear, integrated nano-systems, acoustical MMs, photonics, plasmonics, absorbers / emitters, topological photonics.



# CENTER FOR METAMATERIALS AND INTEGRATED PLASMONICS DUKE UNIVERSITY



David Smith



Willie Padilla

## 20 YEARS OF METAMATERIALS

VOLUME 84, NUMBER 18

PHYSICAL REVIEW LETTERS

1 MAY 2000

### **Composite Medium with Simultaneously Negative Permeability and Permittivity**

D. R. Smith,\* Willie J. Padilla, D. C. Vier, S. C. Nemat-Nasser, and S. Schultz

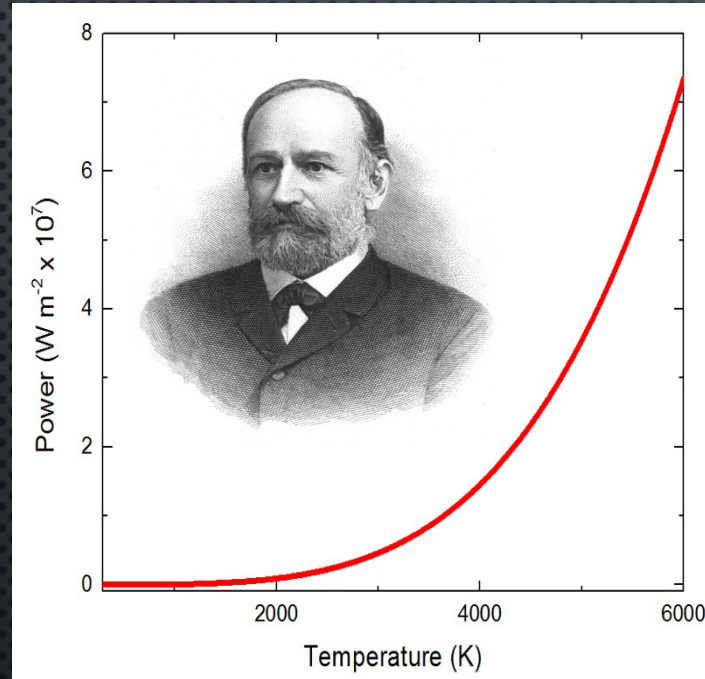
*Department of Physics, University of California, San Diego, 9500 Gilman Drive, La Jolla, California 92093-0319*

(Received 2 December 1999)

We demonstrate a composite medium, based on a periodic array of interspaced conducting nonmagnetic split ring resonators and continuous wires, that exhibits a frequency region in the microwave regime with simultaneously negative values of effective permeability  $\mu_{\text{eff}}(\omega)$  and permittivity  $\varepsilon_{\text{eff}}(\omega)$ . This structure forms a “left-handed” medium, for which it has been predicted that such phenomena as the Doppler effect, Cherenkov radiation, and even Snell’s law are inverted. It is now possible through microwave experiments to test for these effects using this new metamaterial.



# MOTIVATION – BLACKBODY RADIATION



Josef Stefan  
(1835 – 1893)

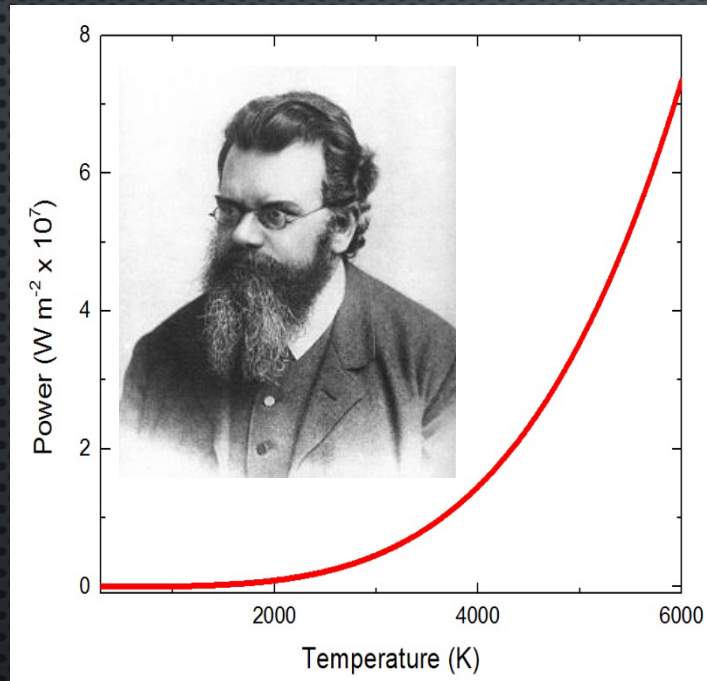
1879 – Total power per unit area emitted at all frequencies by a hot solid was proportional to the fourth power of its absolute temperature  $T$ .

$$M(T) \propto T^4$$





# BLACKBODY RADIATION



Ludwig Boltzmann  
(1844 – 1906)

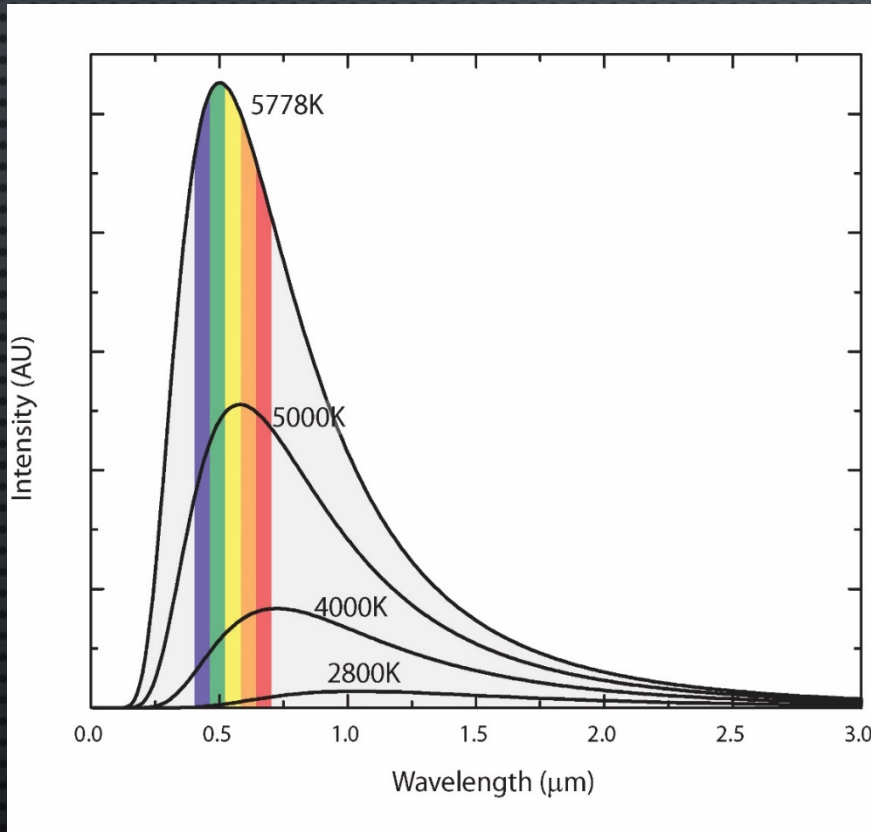
1884 – Derived Stefan's law from Maxwell's equations and thermodynamics.

$$M(T) = \epsilon\sigma T^4$$





# BLACKBODY RADIATION



Max Planck  
(1858 – 1947)

1900 – Derived the blackbody distribution law from statistical mechanics and Maxwell's equations.

$$B(\lambda, T) = \frac{2\pi hc^2}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1}$$





# BLACKBODY RADIATION



Thomas Wedgwood  
(1771 – 1805)

1792 – All the objects in his ovens, regardless of their chemical nature, size, or shape, became red at the same temperature.

Natural materials are limited by the Stefan-Boltzmann law

Engineered materials provide a path forward to overcome SB-law



# WHY DO WE CARE ABOUT THE BLACKBODY?

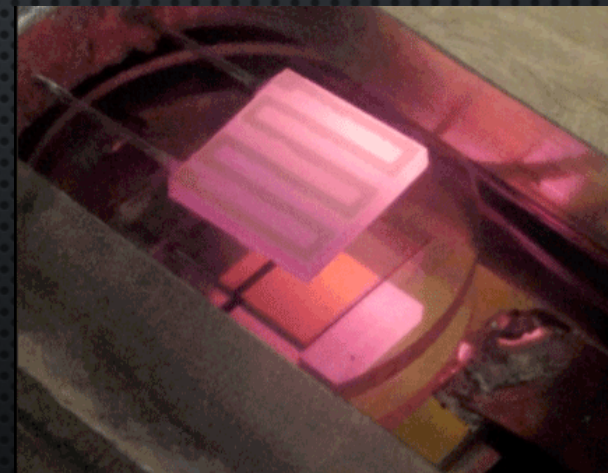
- Controlled Incandescence

- Lighting



- Energy Harvesting

- Thermophotovoltaics





# PHOTOPIC SENSITIVITY OF THE EYE

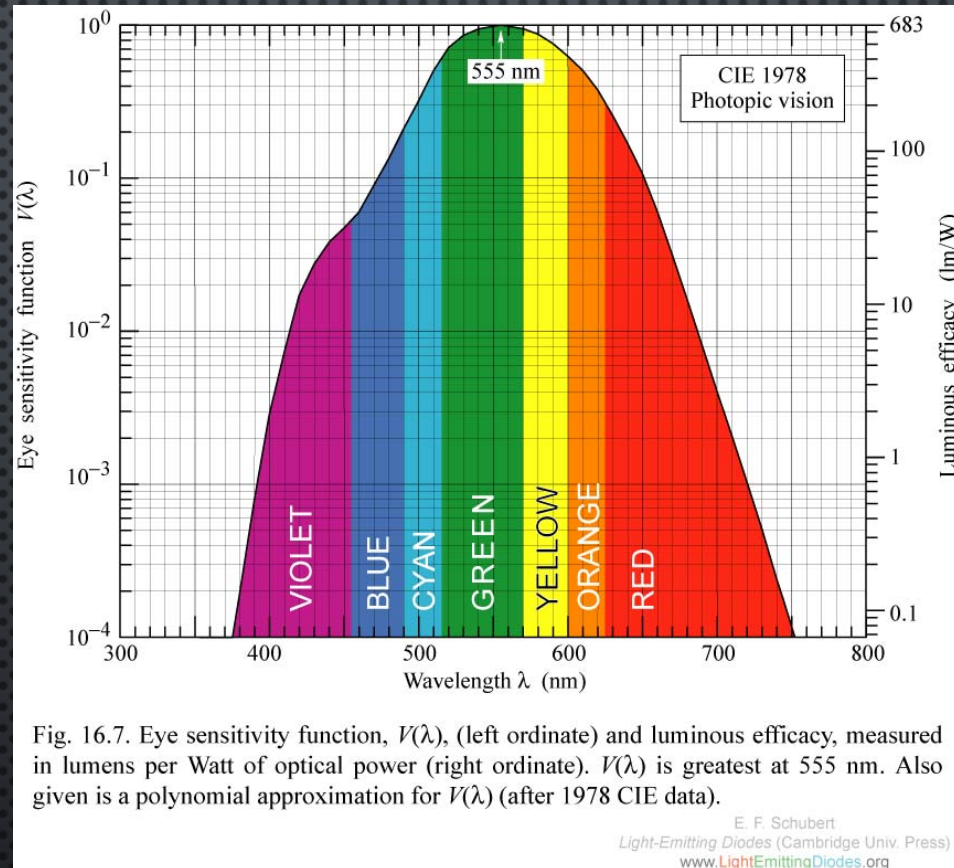


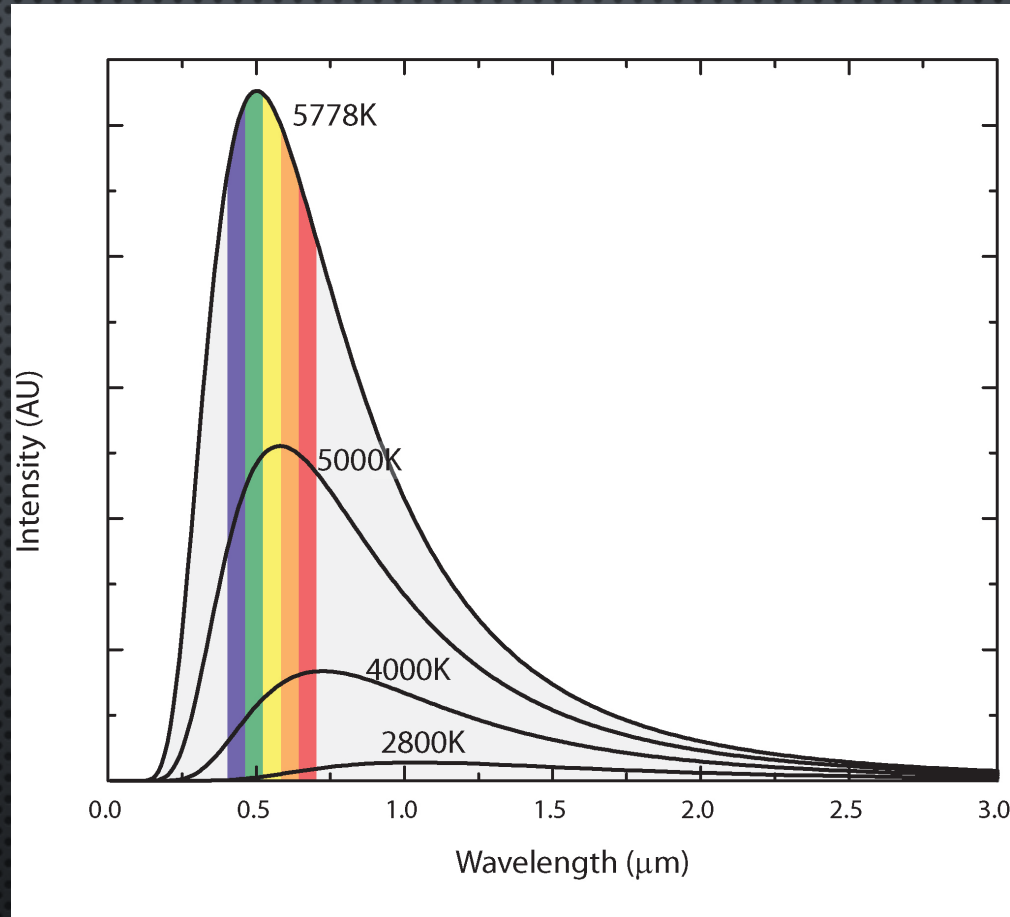
Fig. 16.7. Eye sensitivity function,  $V(\lambda)$ , (left ordinate) and luminous efficacy, measured in lumens per Watt of optical power (right ordinate).  $V(\lambda)$  is greatest at 555 nm. Also given is a polynomial approximation for  $V(\lambda)$  (after 1978 CIE data).

E. F. Schubert  
Light-Emitting Diodes (Cambridge Univ. Press)  
[www.LightEmittingDiodes.org](http://www.LightEmittingDiodes.org)

- Photopic (well-lit conditions) sensitivity peaks at 555nm
- Eye sensitivity shifts to shorter wavelengths for low lighting
- CIE 1978 polynomial is standard fit used for lighting



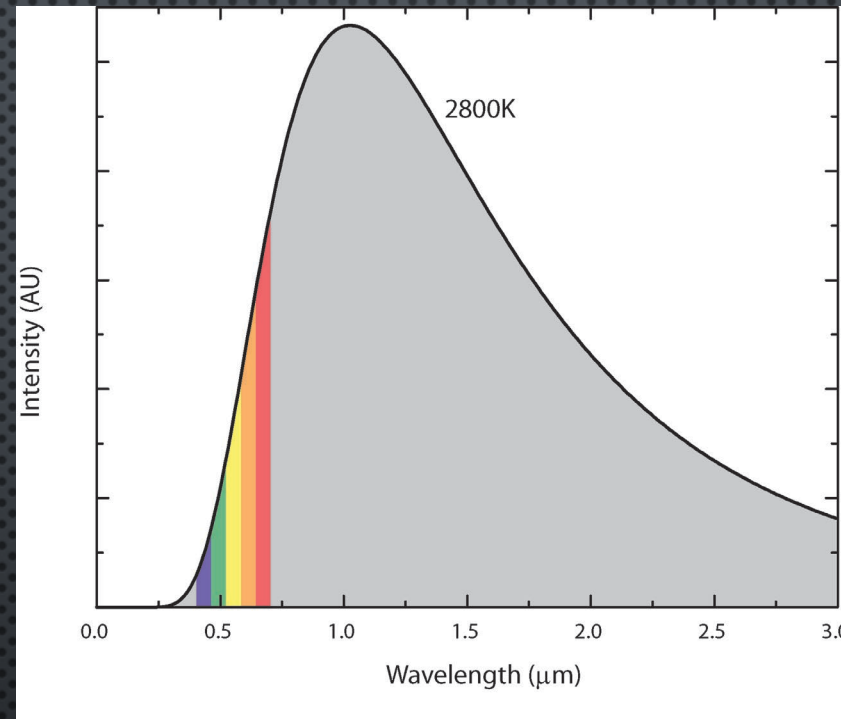
# PHOTOPIC SENSITIVITY OF THE EYE



- Human eye optimized for sunlight
- Sun is a blackbody at  $\sim 5800\text{K}$



# PHOTOPIC SENSITIVITY OF THE EYE



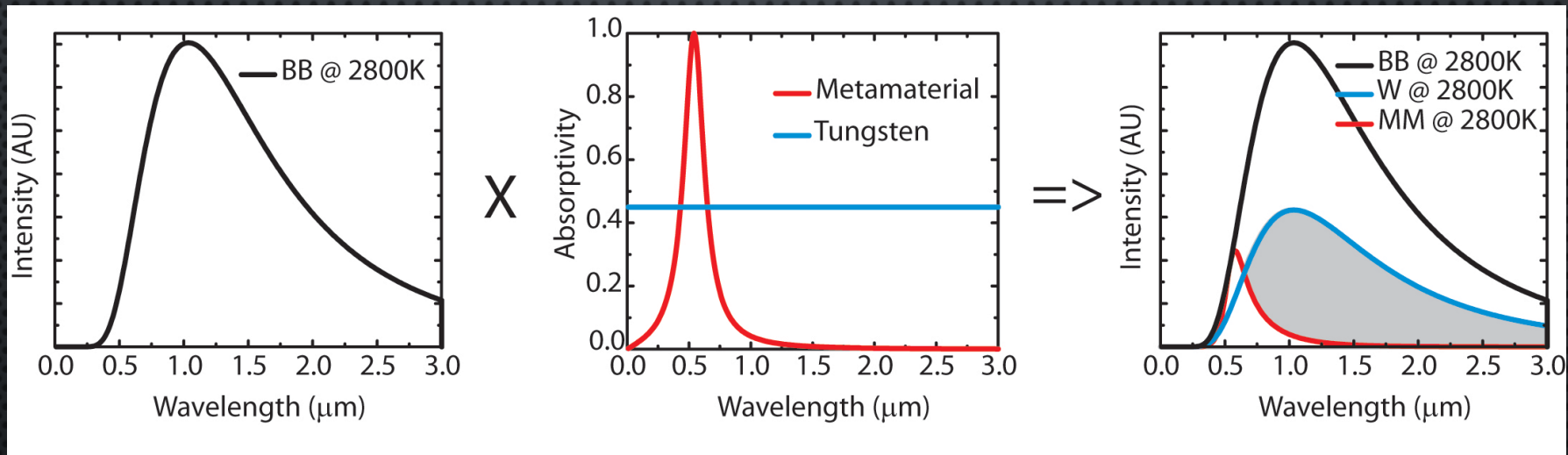
- Tungsten light bulbs operate at 2800K
- Black body peaks in the near infrared
- Generates waste heat
- Emissivity of tungsten is ~45%



# HOW TO CONTROL EMISSION WITH METAMATERIALS

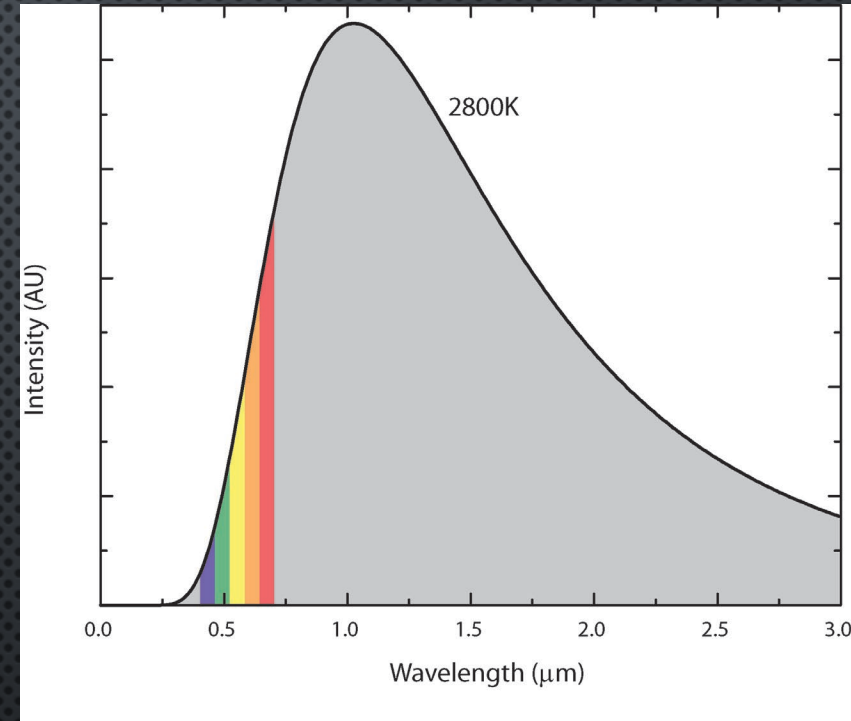
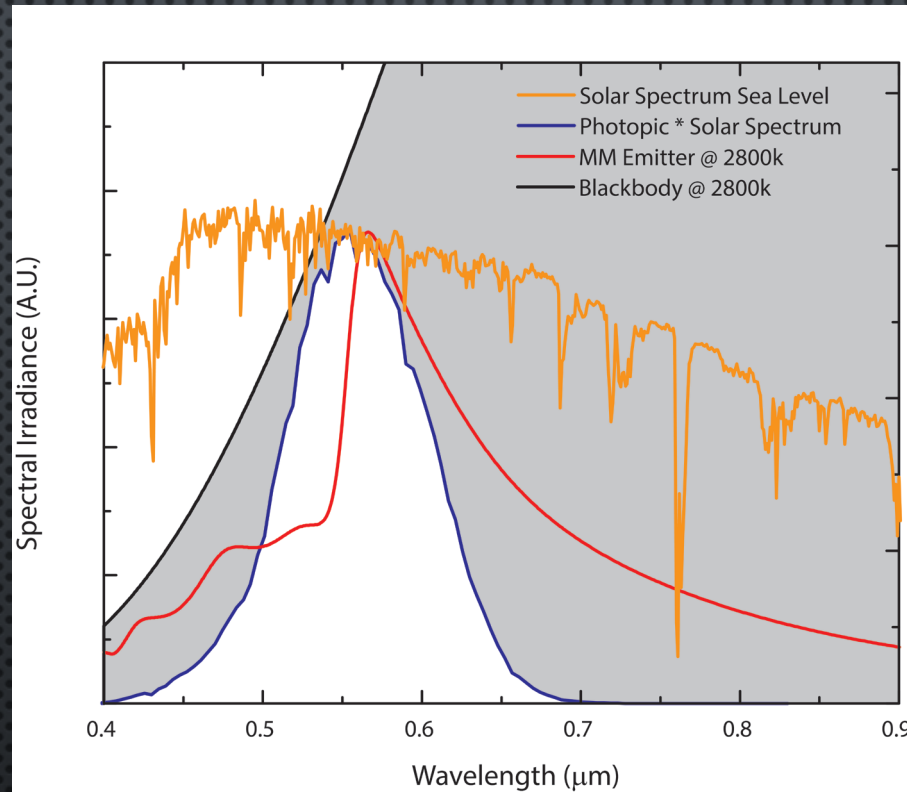
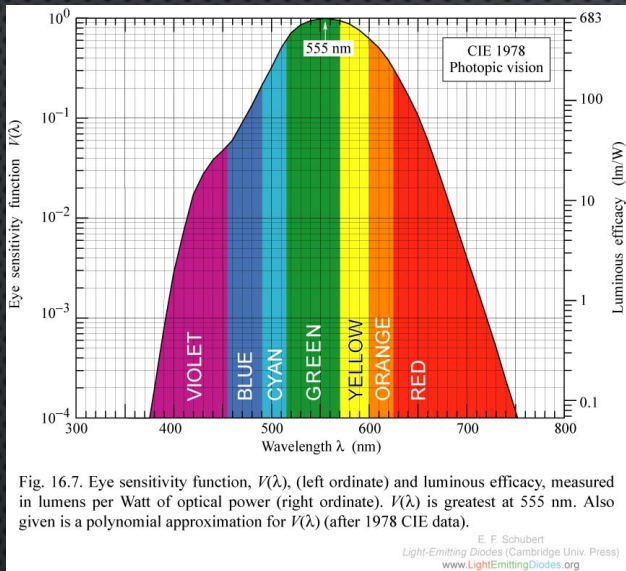
Kirchoff's law of thermal radiation - 1859

*At thermal equilibrium, the emissivity of a body or surface equals its absorptivity*



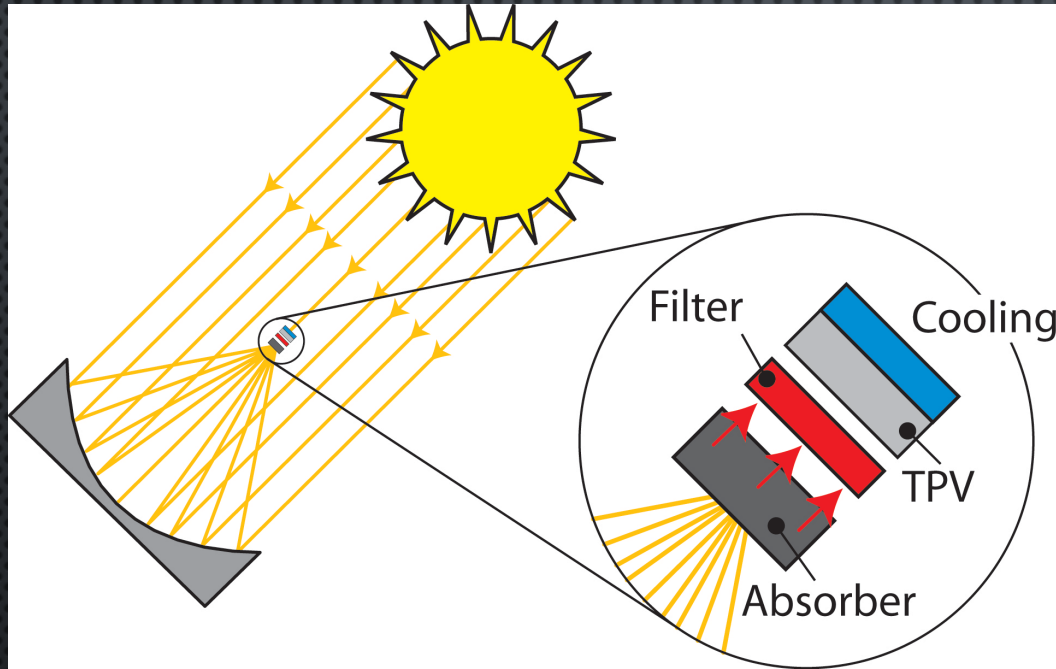


# METAMATERIAL LIGHTING

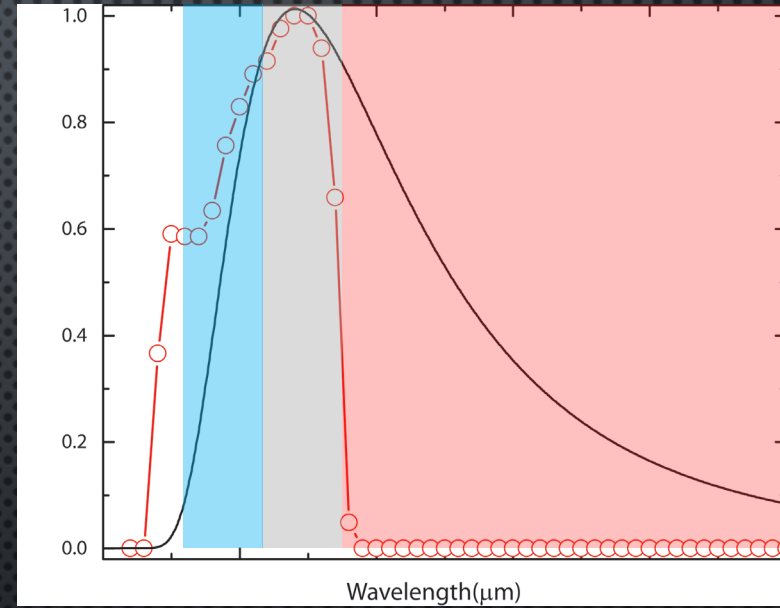




# ENERGY HARVESTING - THERMOPHOTOVOLTAICS

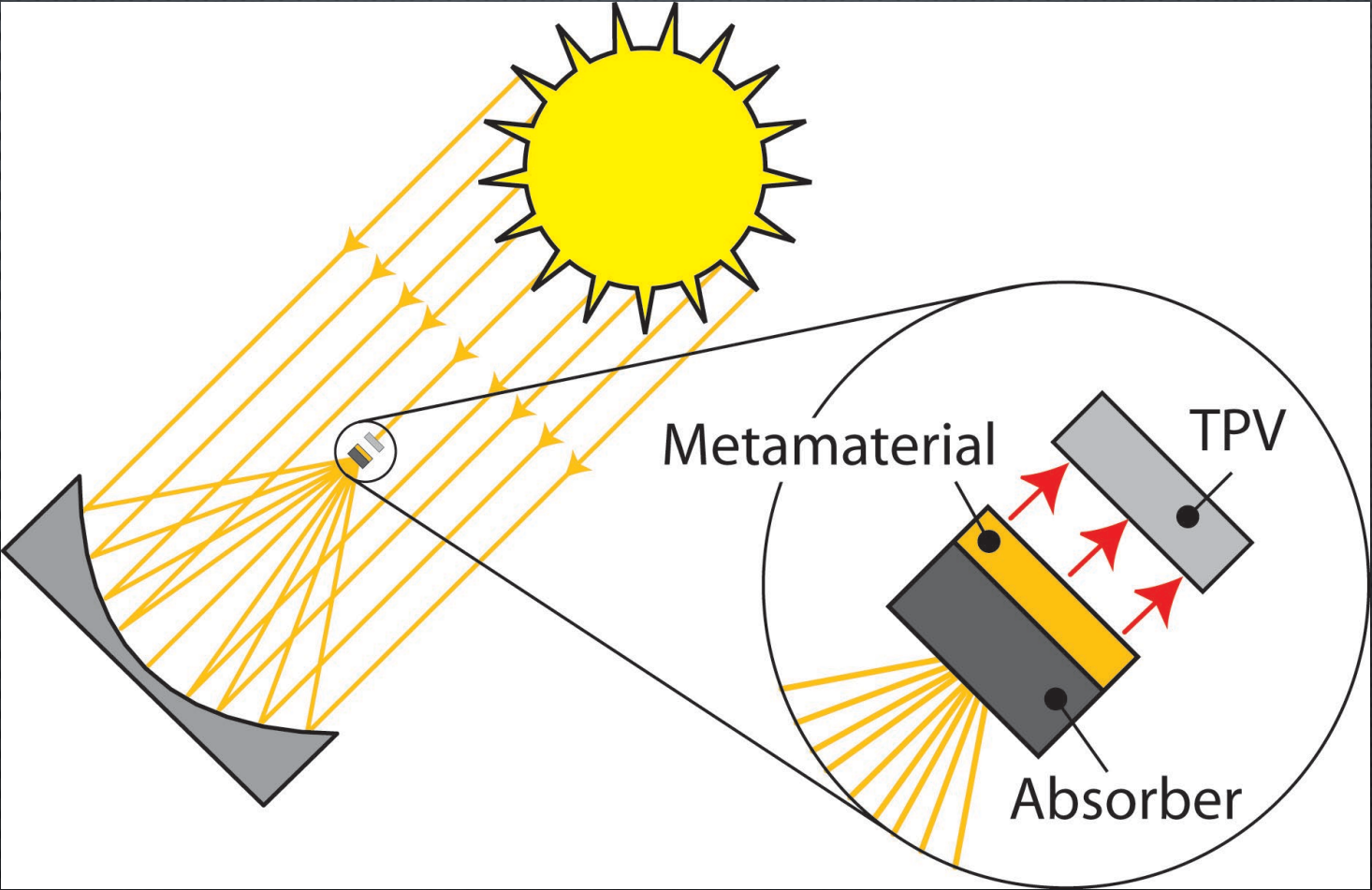


External Quantum Efficiency



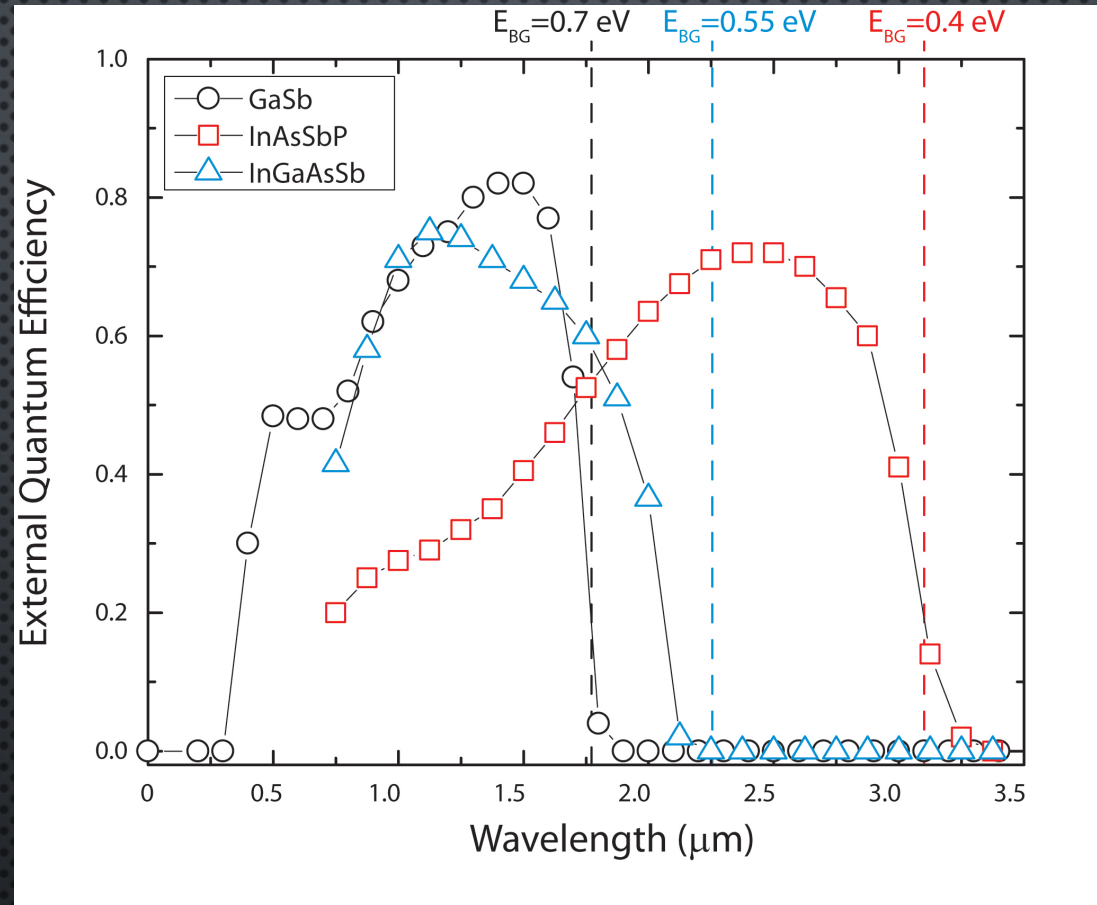


# ENERGY HARVESTING





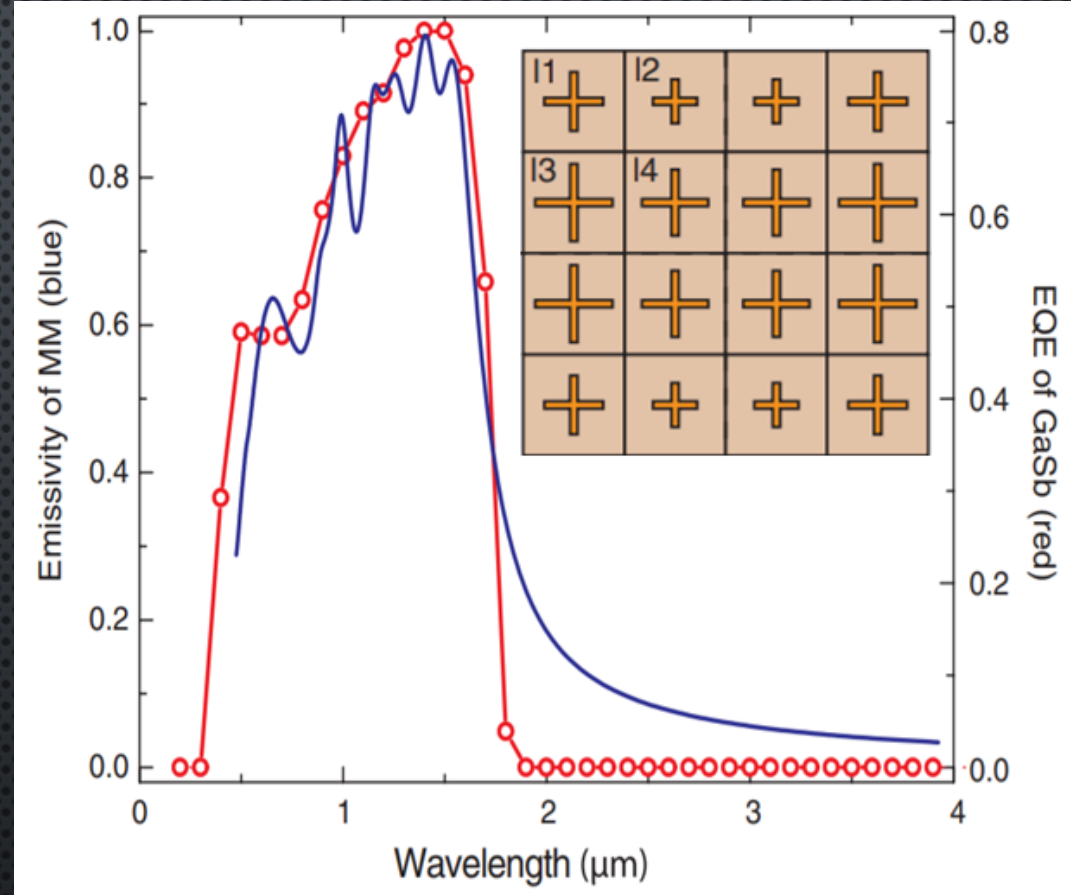
# ENERGY HARVESTING



Material	Band Gap Energy (eV) @300K	Wavelength (nm)
SiC	2.86	434
Si	1.12	1107
GaSb	0.7	1771
Ge	0.67	1851
InGaAsSb	0.55	2254
InAsSbP	0.4	3100
PbS	0.37	3351



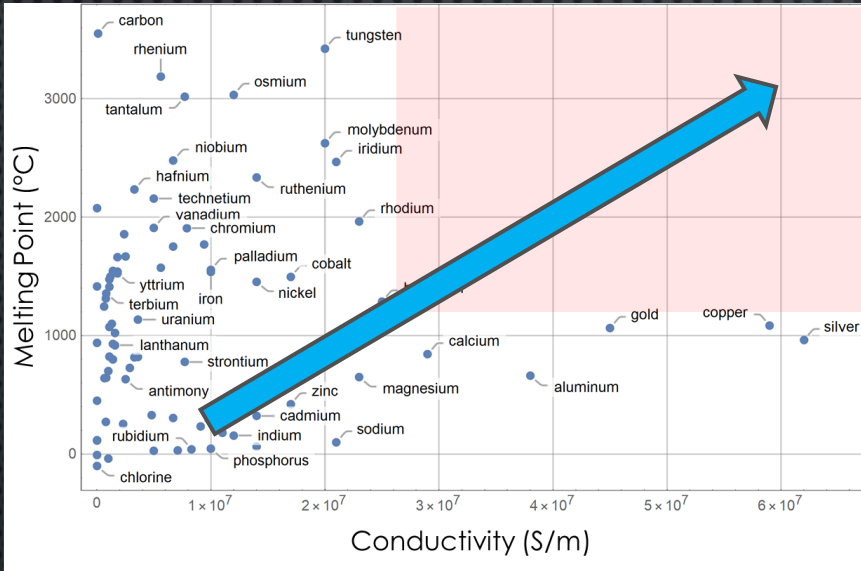
# TAMING THE BLACKBODY



$$M(T) = \varepsilon\sigma T^4$$

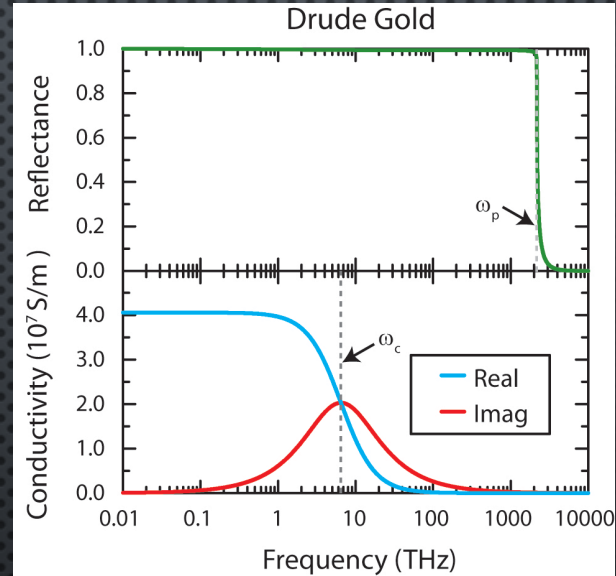


# METAMATERIAL LIMITATIONS



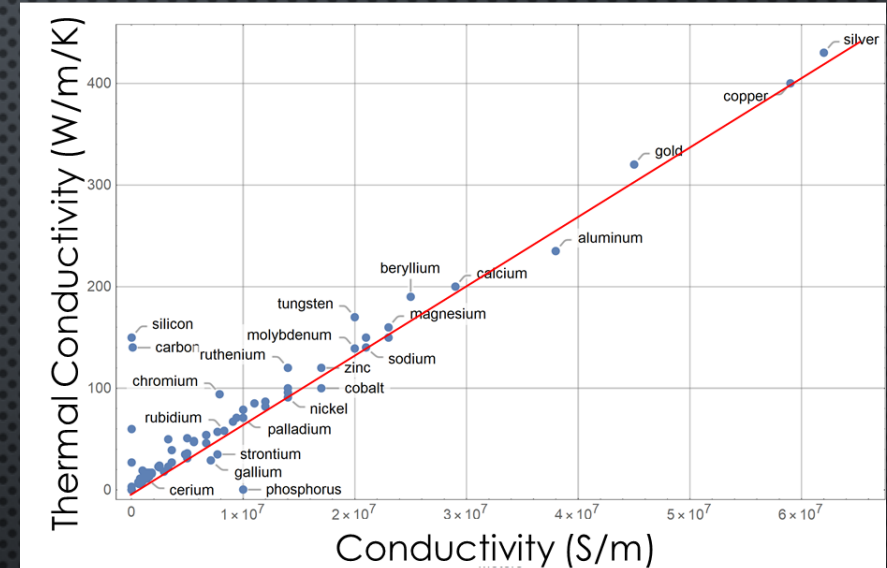
Low Melting Temperatures

$$M(T) = \varepsilon\sigma T^4$$



Ohmic Losses

$$\sigma(\omega) = \frac{\sigma_0}{1 - i\omega\tau}$$

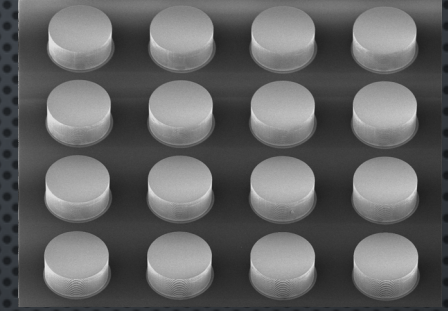
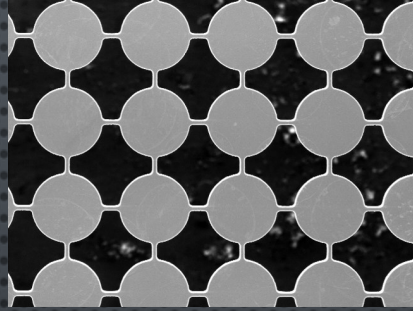
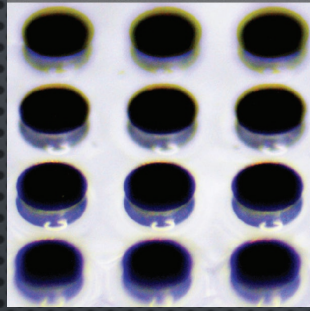
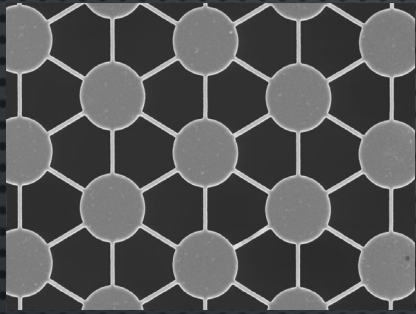


High Thermal Conductivities

$$\kappa = \sigma L T$$



# FUNDAMENTALLY DIFFERENT APPROACH



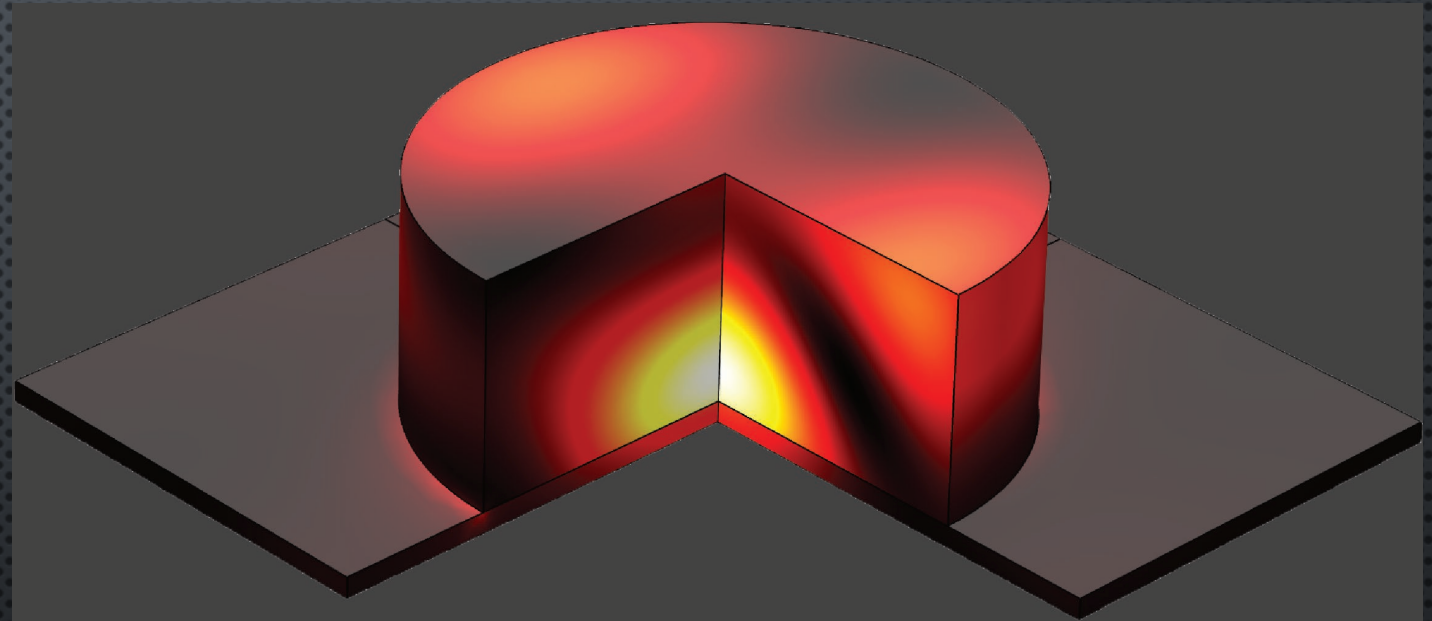
1. EM response determined by geometrical parameters
2. Independent and direct control of  $\epsilon(\omega)$  and  $\mu(\omega)$
3. Multifunctional properties
4. EM response comes from the 'meta-atom', not from the array

New problems emerge...



# OUTLINE

- **ALL-DIELECTRIC METASURFACES**
- MACHINE LEARNING
- INVERSE DESIGN
- ARTIFICIAL “INTELLIGENCE”
- CONCLUSION





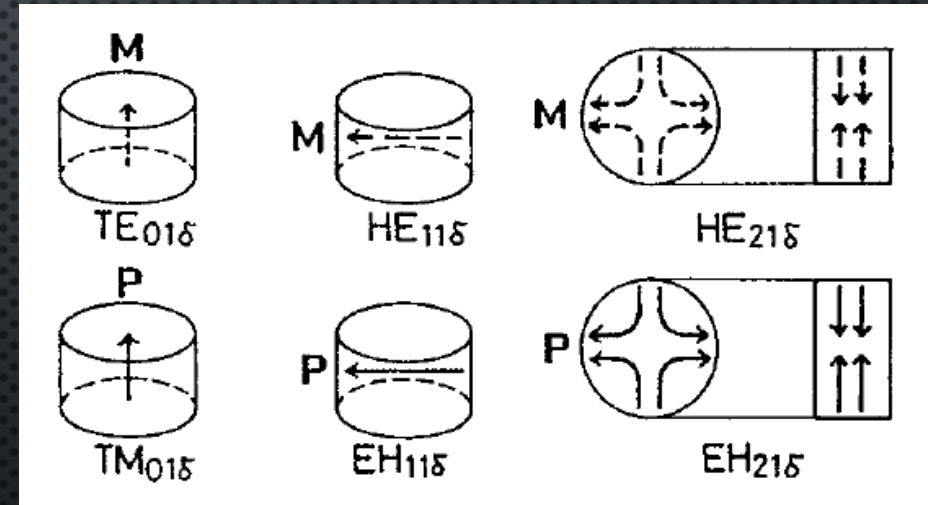
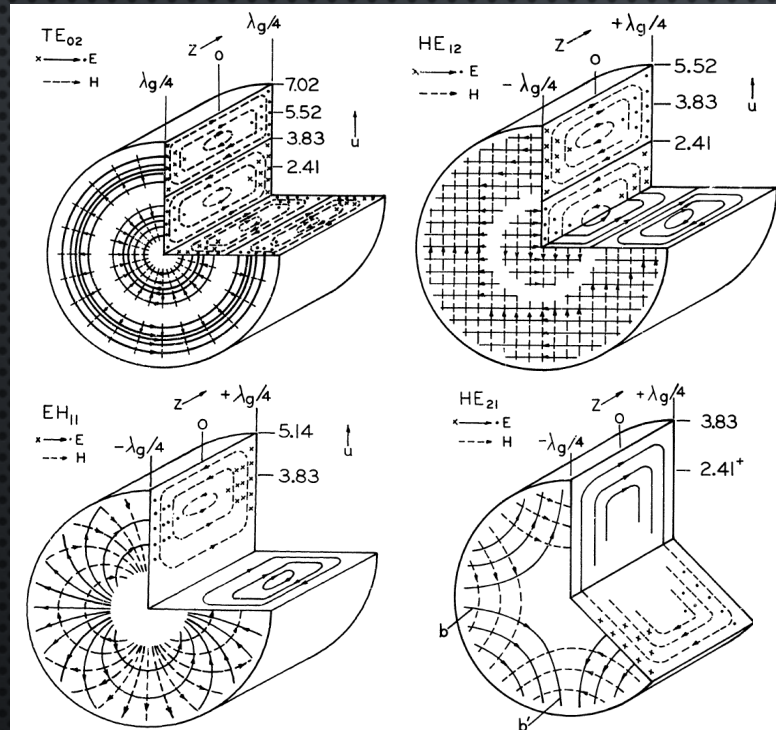
# DIELECTRIC WAVEGUIDES AND RESONATORS



Elias Snitzer



Yoshio Kobayashi



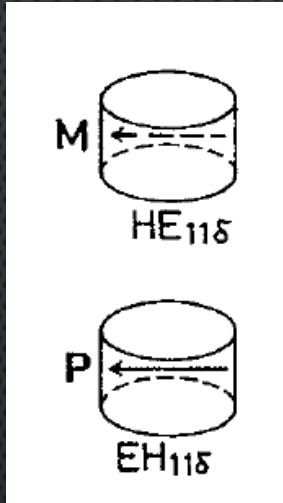
Y. Kobayashi and S. Tanaka, "Resonant Modes of a Dielectric Rod Resonator Short-Circuited at Both Ends by Parallel Conducting Plates," IEEE Trans. Microw. Theory Techn. 28, 1077–1085 (1980).

E. Snitzer, "Cylindrical dielectric waveguide modes," J. Opt. Soc. Amer. 51, 491–498 (1961).



# DIELECTRIC WAVEGUIDES AND RESONATORS

Z  
↑



HE Mode is an approximate TM mode

$H_z / E_z \ll 1$  for the HE Mode

EH Mode is an approximate TE mode

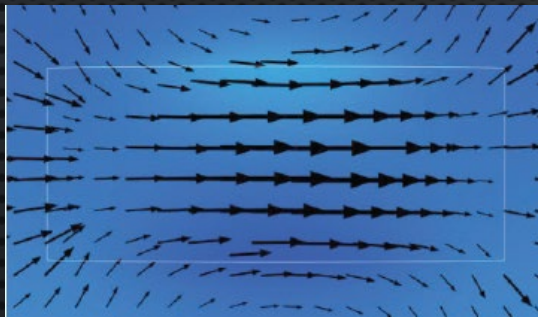
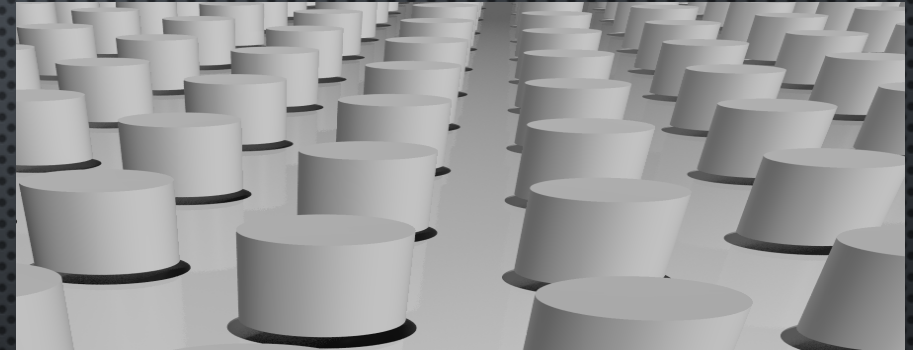
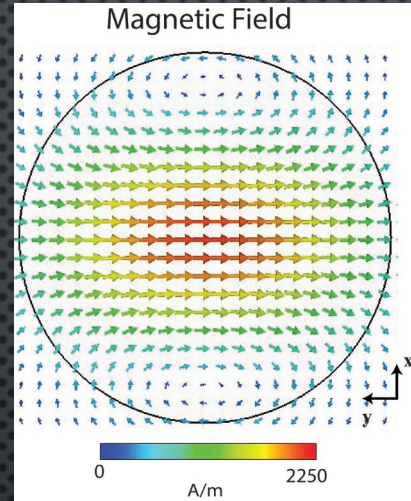
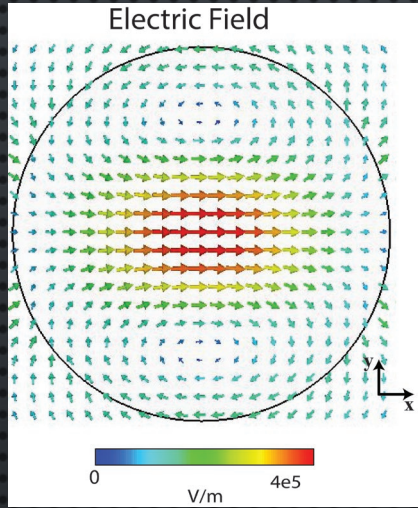
$E_z / H_z \ll 1$  for the EH Mode

Field variation within the cylinder is denoted by three indices, i.e.  $HE_{nml}$  and  $EH_{nml}$

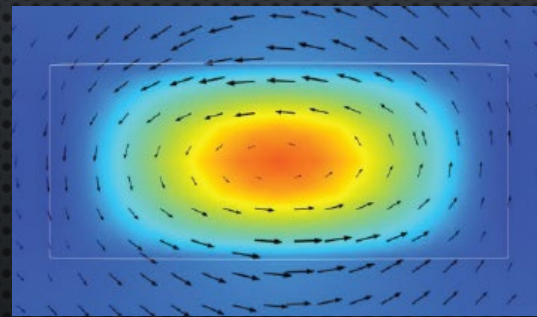
- $n$  azimuthal variation (form of  $\sin n$  and  $\cos n$ )
- $m$  denotes the field variation along the radial direction
- $l$  along the  $z$ -axis



# ELECTRIC AND MAGNETIC DIPOLE MODES



EH – Even Mode



HE – Odd Mode



# THEORY OF DIELECTRIC METAMATERIAL ABSORBERS

$$\underline{EH}_{111}$$

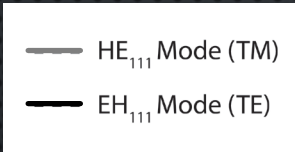
$$J_1(k_r r) = 0$$

$$\tan\left(\frac{k_z h}{2}\right) = \frac{k_{z0}}{k_z}$$

$$\underline{HE}_{111}$$

$$k_z h = \pi$$

$$\left[ \frac{J_1'(u)}{uJ_1(u)} + \frac{K_1'(v)}{vK_1(v)} \right] \left[ k_0^2 \varepsilon_{1r} \frac{J_1'(u)}{uJ_1(u)} + k_0^2 \frac{K_1'(v)}{vK_1(v)} \right] = k_z^2 \left( \frac{1}{u^2} + \frac{1}{v^2} \right)^2$$

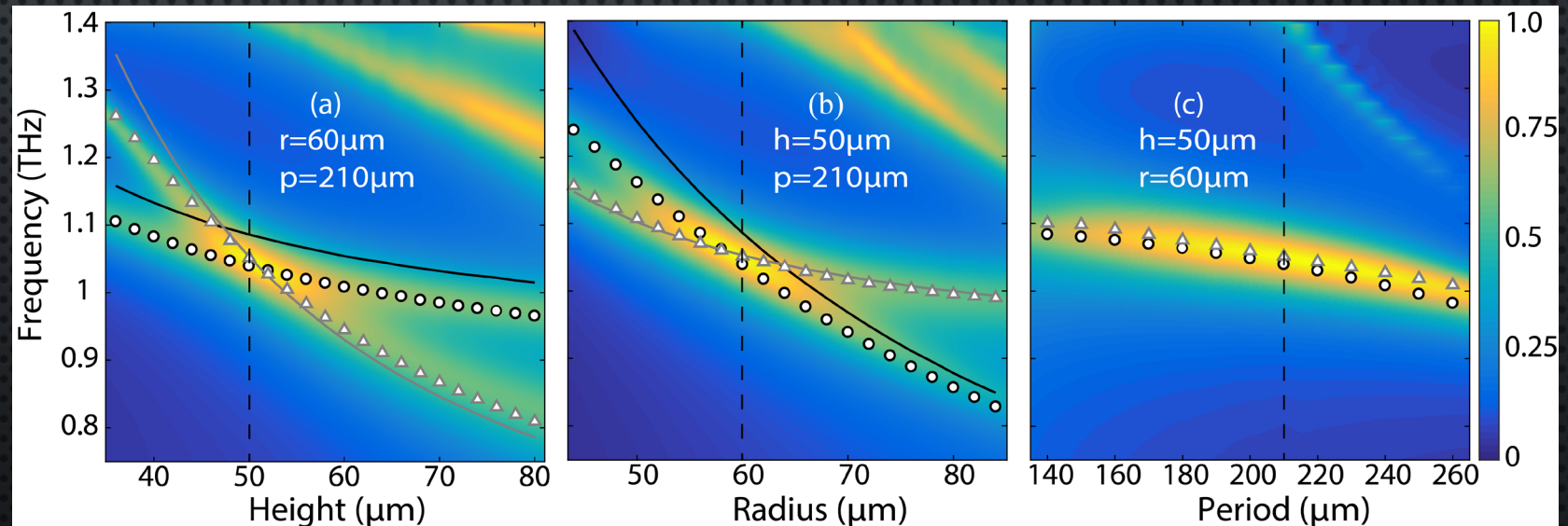


$$u = k_r r$$

$$v = k_r r_0$$

$J_1'(u)$  1<sup>st</sup> order Bessel function

$K_1'(v)$  1<sup>st</sup> order Modified Hankel fnc

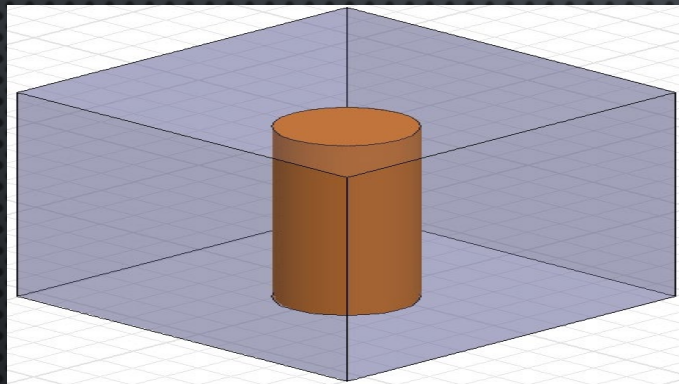




# DEGENERATE CRITICAL COUPLED MODE THEORY

$$A(\omega) = \sum_{j=1}^2 \frac{2\gamma_j \delta_j}{(\omega - \omega_{0,j})^2 + (\gamma_j + \delta_j)^2}$$

$\delta$  Material loss rate  
 $\gamma$  Radiative loss rate  
 $\omega_0$  Resonant frequency



Degenerate  $\omega_{0,1} = \omega_{0,2}$

Critical  $\delta = \gamma$

$$\tilde{\omega} = \omega_1 - i\omega_2 = \omega_1 - i(\gamma + \delta)$$

$$A(\omega_0) \geq 49.0\% \quad \text{for} \quad \frac{3}{4} \leq \frac{\delta}{\gamma} \leq \frac{4}{3}$$

Mode	Analytical $\omega_0$ (THz)	Simulated $\omega_0$ (THz)	$\gamma$ ( $\times 10^9$ 1/s)	$\delta$ ( $\times 10^9$ 1/s)
EH <sub>111</sub>	1.086	1.0440	21.7	22.1
HE <sub>111</sub>	1.053	1.0512	28.1	26.1

- Jessica R. Piper, Victor Liu, and Shanhui Fan, *Total absorption by degenerate critical coupling*, Applied Physics Letters, **104**, 251110 (2014)
- Xianshun Ming, Xinyu Liu, Liqun Sun, and Willie J. Padilla, *Degenerate critical coupling in all-dielectric metasurface absorbers*, Optics Express 25, 24658 (2017)



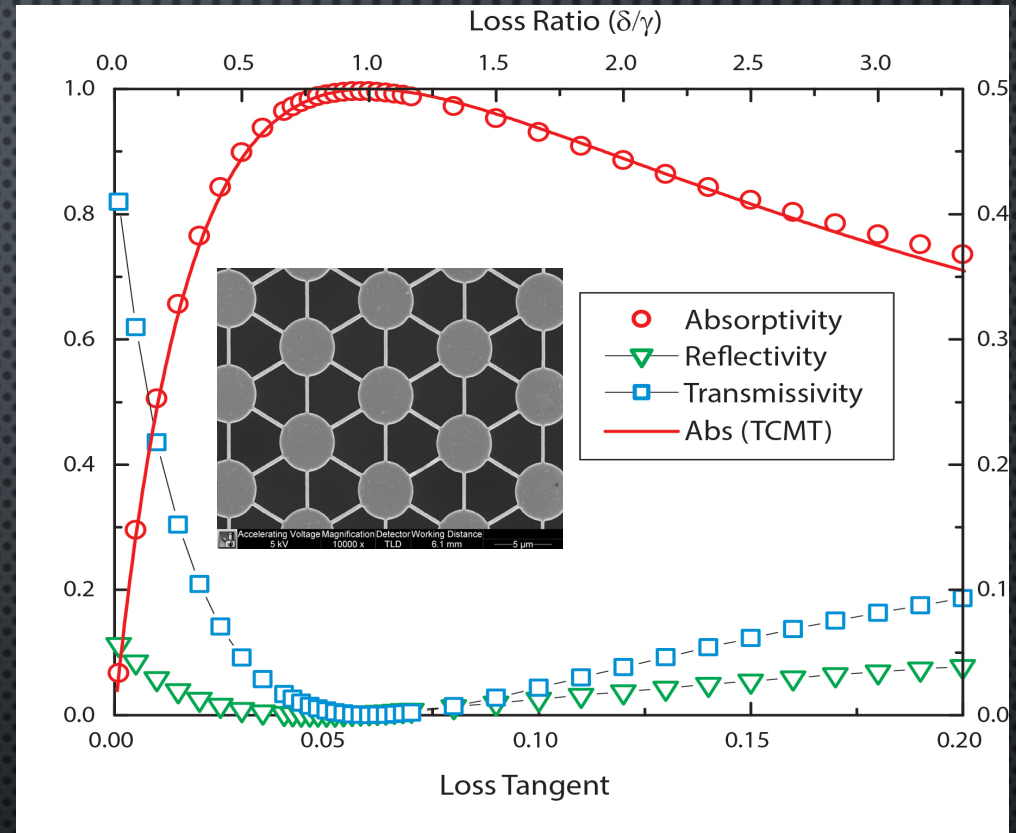
# DESIGNER ALL-DIELECTRIC ABSORBERS

## Absorber Design Rules

1. Operational wavelength  $\lambda_0$
2. Use high index dielectric  $n$
3. Geometry  $r = 0.61 \frac{\lambda_0}{\sqrt{n^2-1}}$ ;  $h = \frac{\lambda_0}{2n}$
4. Periodicity  $2r < p < \lambda$   $r, h, p \rightarrow \gamma$
5. Chose material loss  $\delta = \gamma$

$$A(\delta/\gamma) = 4 \frac{\delta/\gamma}{1 + (\delta/\gamma)^2 + 2\delta/\gamma}$$

$$\frac{r}{h} = 1.22 \frac{n}{\sqrt{n^2-1}} \approx 1.22$$



## Silicon Drude Model

$$\omega_p = 7.3 \times 10^{13} \text{ } 2\pi \times \text{THz}$$

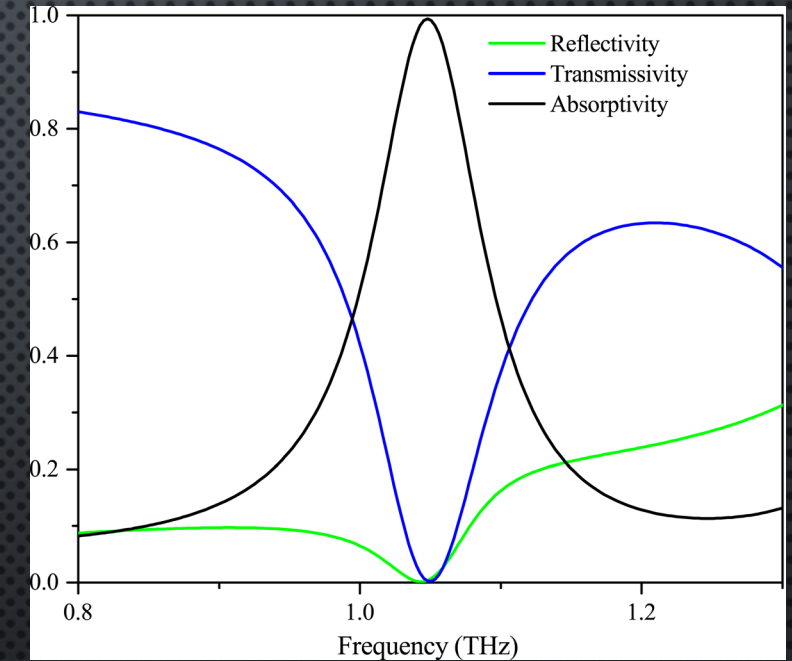
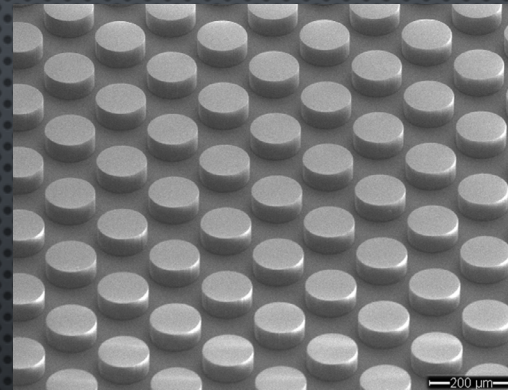
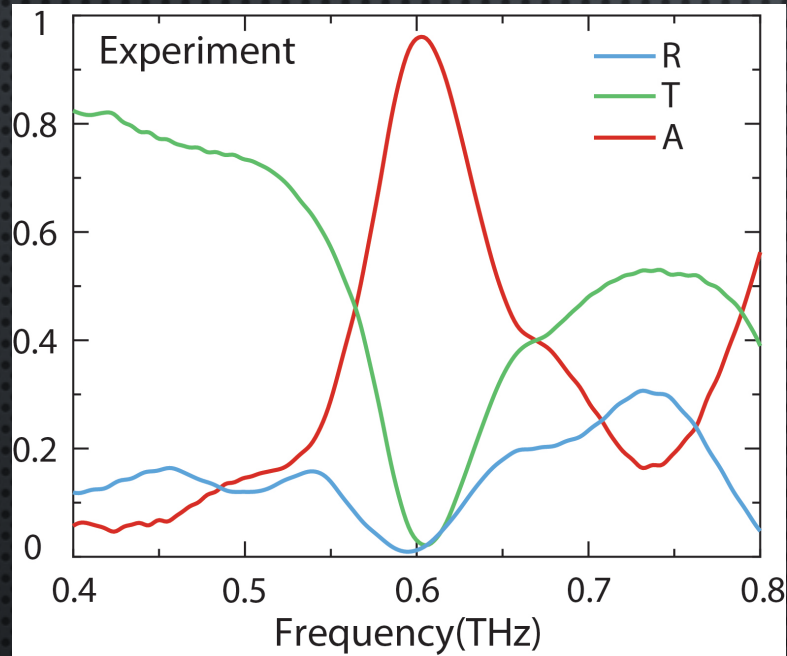
$$\gamma = 1.0 \times 10^{13} \text{ } 2\pi \times \text{THz}$$

$$\epsilon_\infty = 11.7$$

$$\tan \delta = 0.06$$



# DIELECTRIC METAMATERIAL ABSORBERS





# THZ ALL-DIELECTRIC ABSORBER

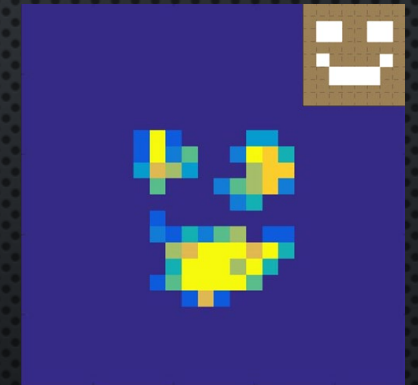
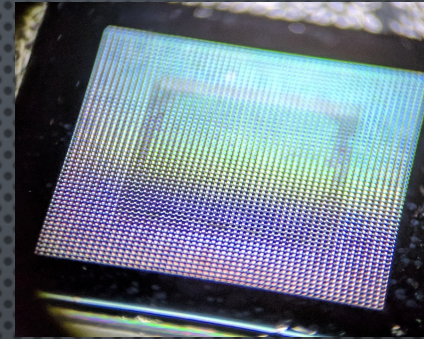
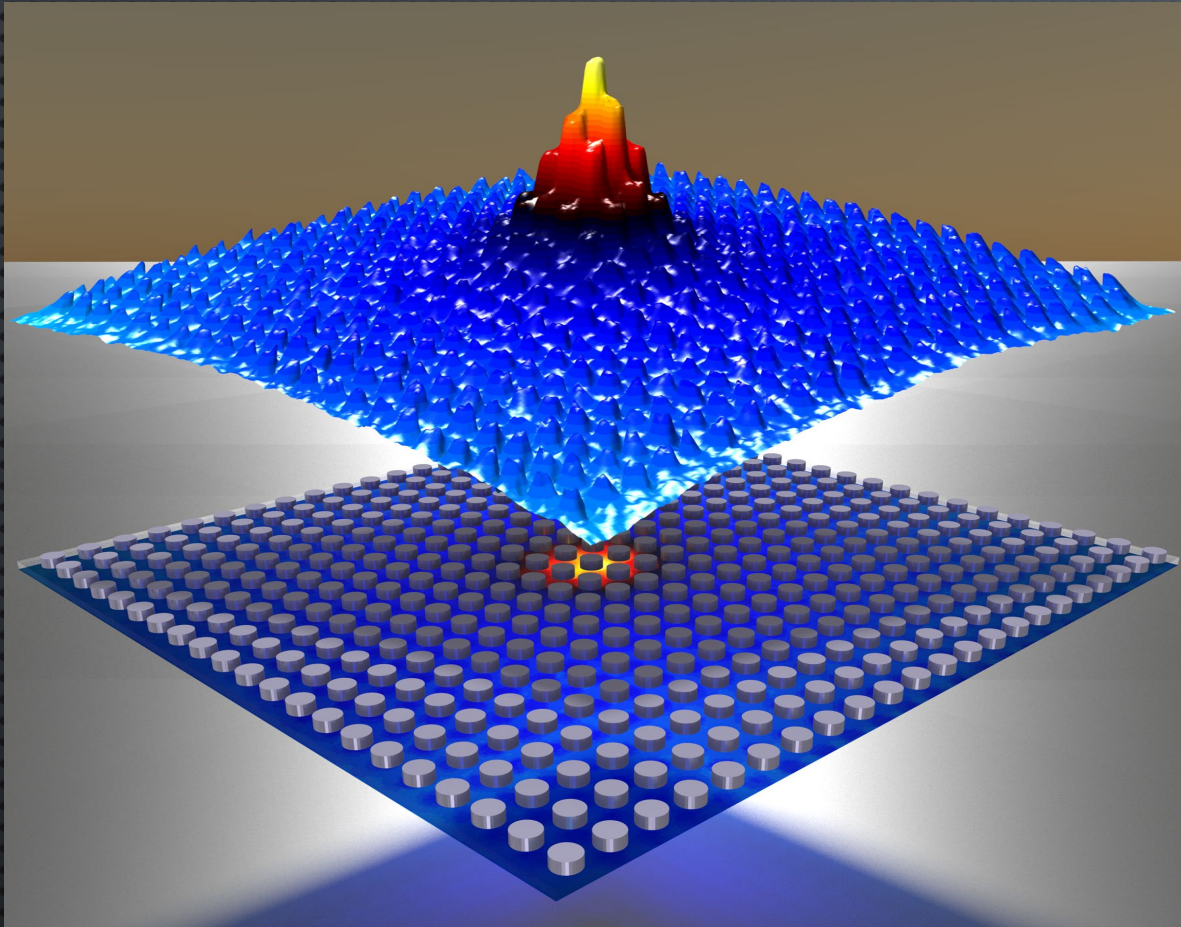
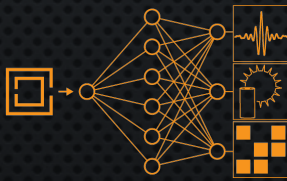
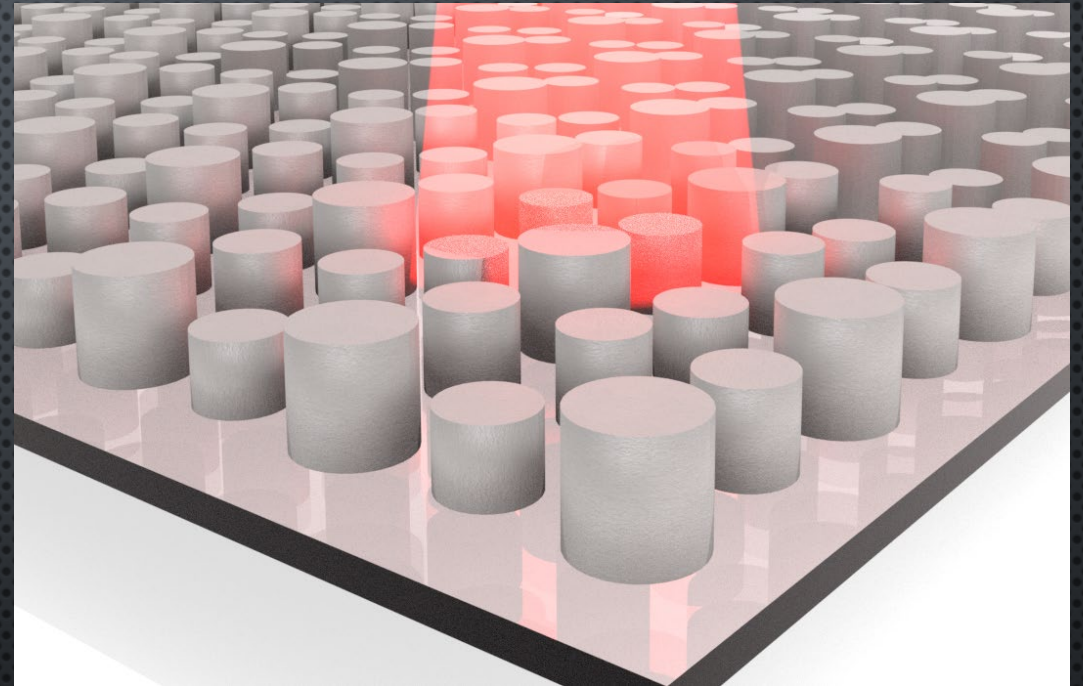


Image – Kebin Fan



# OUTLINE

- ALL-DIELECTRIC METASURFACES
- **MACHINE LEARNING**
- INVERSE DESIGN
- ARTIFICIAL “INTELLIGENCE”
- CONCLUSION





# NEURAL NETWORK ARCHITECTURES

## A mostly complete chart of Neural Networks

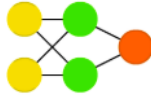
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- Input Cell
- Backfed Input Cell
- △ Noisy Input Cell
- Hidden Cell
- Probabilistic Hidden Cell
- △ Spiking Hidden Cell
- Capsule Cell
- Output Cell
- Match Input Output Cell
- Recurrent Cell
- Memory Cell
- △ Gated Memory Cell
- Kernel
- Convolution or Pool

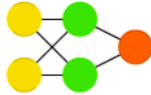
Perceptron (P)



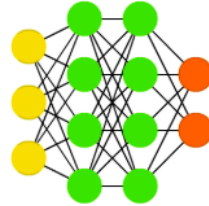
Feed Forward (FF)



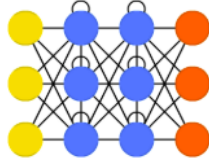
Radial Basis Network (RBF)



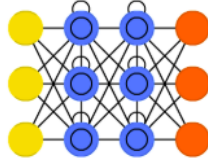
Deep Feed Forward (DFF)



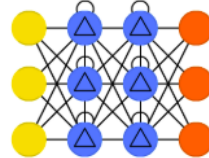
Recurrent Neural Network (RNN)



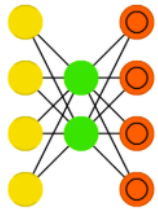
Long / Short Term Memory (LSTM)



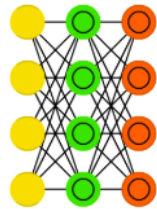
Gated Recurrent Unit (GRU)



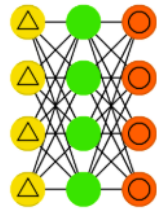
Auto Encoder (AE)



Variational AE (VAE)



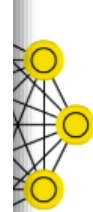
Denosing AE (DAE)



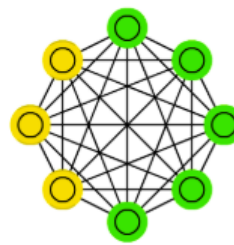
Sparse AE (SAE)



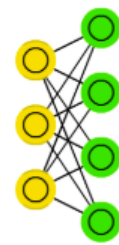
Hopfield Network (HN)



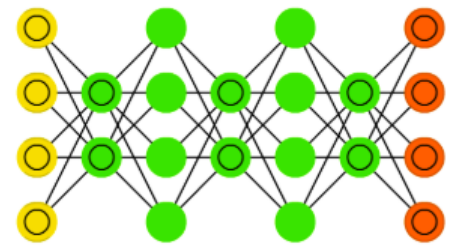
Boltzmann Machine (BM)



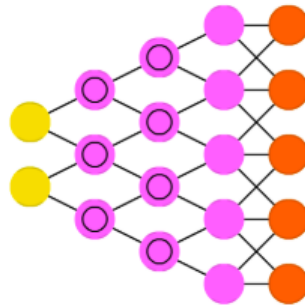
Restricted BM (RBM)



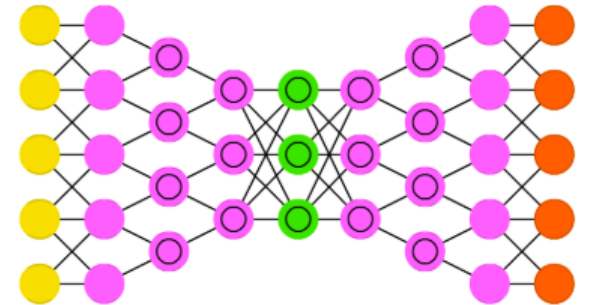
Deep Belief Network (DBN)



Deconvolutional Network (DN)



Deep Convolutional Inverse Graphics Network (DCIGN)



Markov Chain (MC)

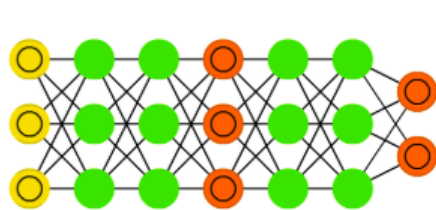
Hopfield Network (HN)

Boltzmann Machine (BM)

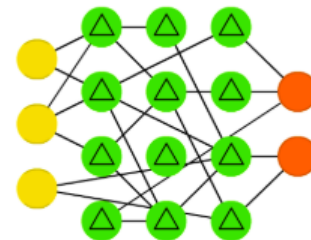
Restricted BM (RBM)

Deep Belief Network (DBN)

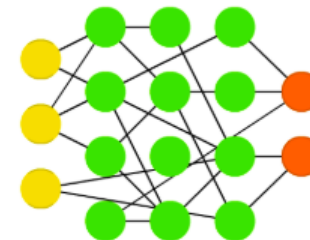
Generative Adversarial Network (GAN)



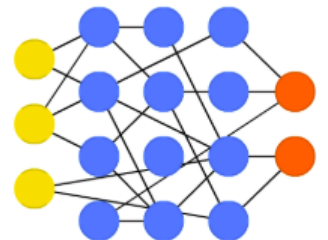
Liquid State Machine (LSM)



Extreme Learning Machine (ELM)

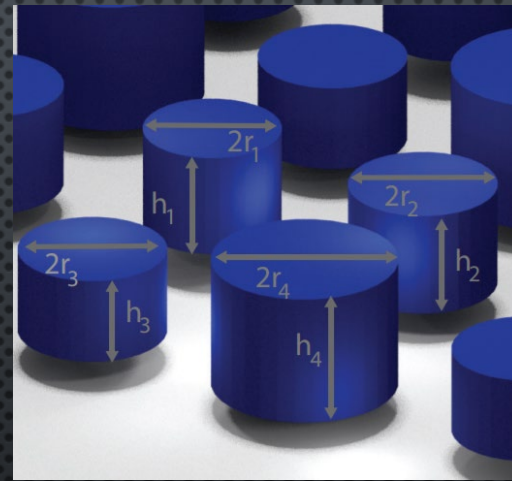
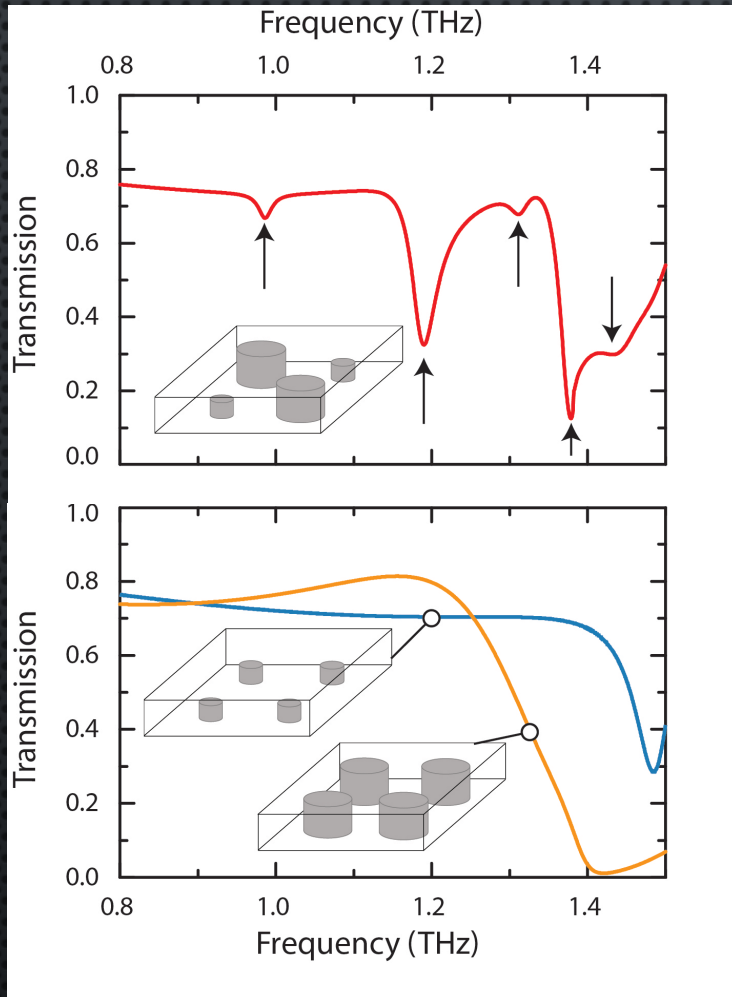


Echo State Network (ESN)





# MACHINE LEARNING FOR ACCELERATED METASURFACE DESIGN



Drude Model

$$\omega_p = 7.3 \times 10^{13} \text{ } 2\pi \times \text{THz}$$

$$\gamma = 1.0 \times 10^{13} \text{ } 2\pi \times \text{THz}$$

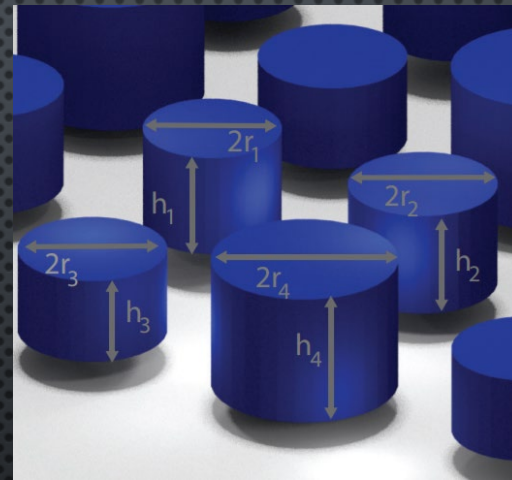
$$\epsilon_\infty = 11.7$$

r (μm)	h (μm)
42.0	30.0
42.8	32.0
43.7	34.0
44.5	36.0
45.3	38.0
46.2	40.0
47.0	42.5
47.8	44.0
48.6	46.0
49.5	48.0
50.4	50.0
51.2	52.0
52.0	55.0



# MACHINE LEARNING FOR ACCELERATED METASURFACE DESIGN

- $13^8$  total permutations  $\sim$  816 million
- $\sim$ 2200 years of compute time
- 18,000 electromagnetic simulations for the training set
- 3,000 electromagnetic simulations reserved for validation set



Drude Model

$$\omega_p = 7.3 \times 10^{13} \text{ } 2\pi \times \text{THz}$$

$$\gamma = 1.0 \times 10^{13} \text{ } 2\pi \times \text{THz}$$

$$\epsilon_\infty = 11.7$$

r ( $\mu\text{m}$ )	h ( $\mu\text{m}$ )
42.0	30.0
42.8	32.0
43.7	34.0
44.5	36.0
45.3	38.0
46.2	40.0
47.0	42.5
47.8	44.0
48.6	46.0
49.5	48.0
50.4	50.0
51.2	52.0
52.0	55.0



# NEURAL NETWORK ARCHITECTURE

Input Geometry

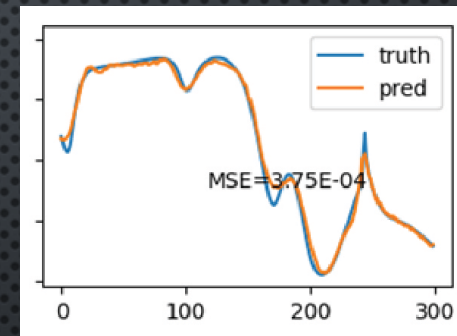
$$\begin{Bmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \\ r_1 \\ r_2 \\ r_3 \\ r_4 \end{Bmatrix}$$


Black Box

$$f(h_1, h_2, h_3, h_4, r_1, r_2, r_3, r_4)$$



Predicted Spectra



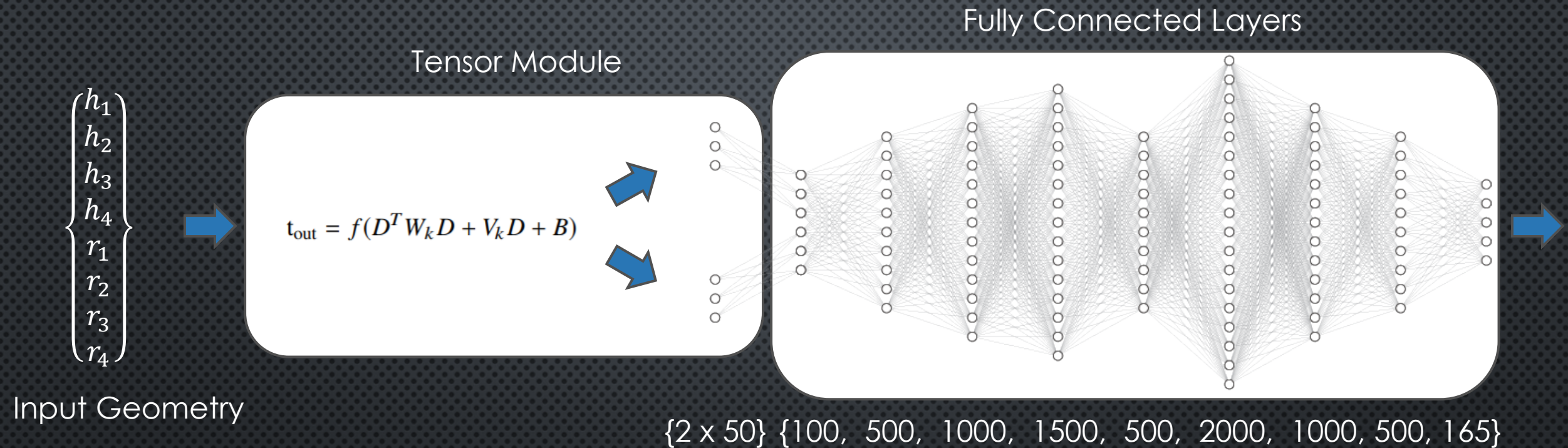
8



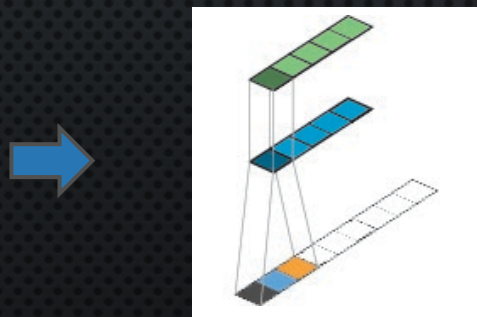
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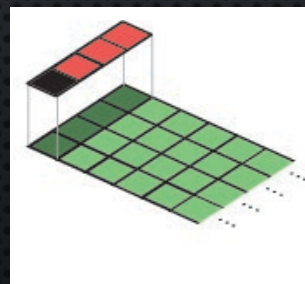
# NEURAL NETWORK ARCHITECTURE – TENSOR LAYER



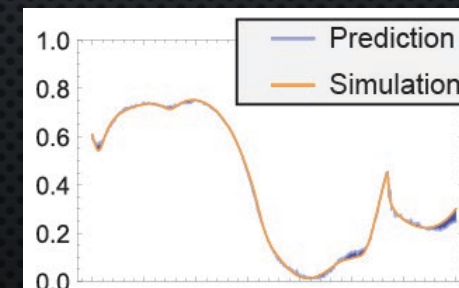
Transpose Convolution



Convolution

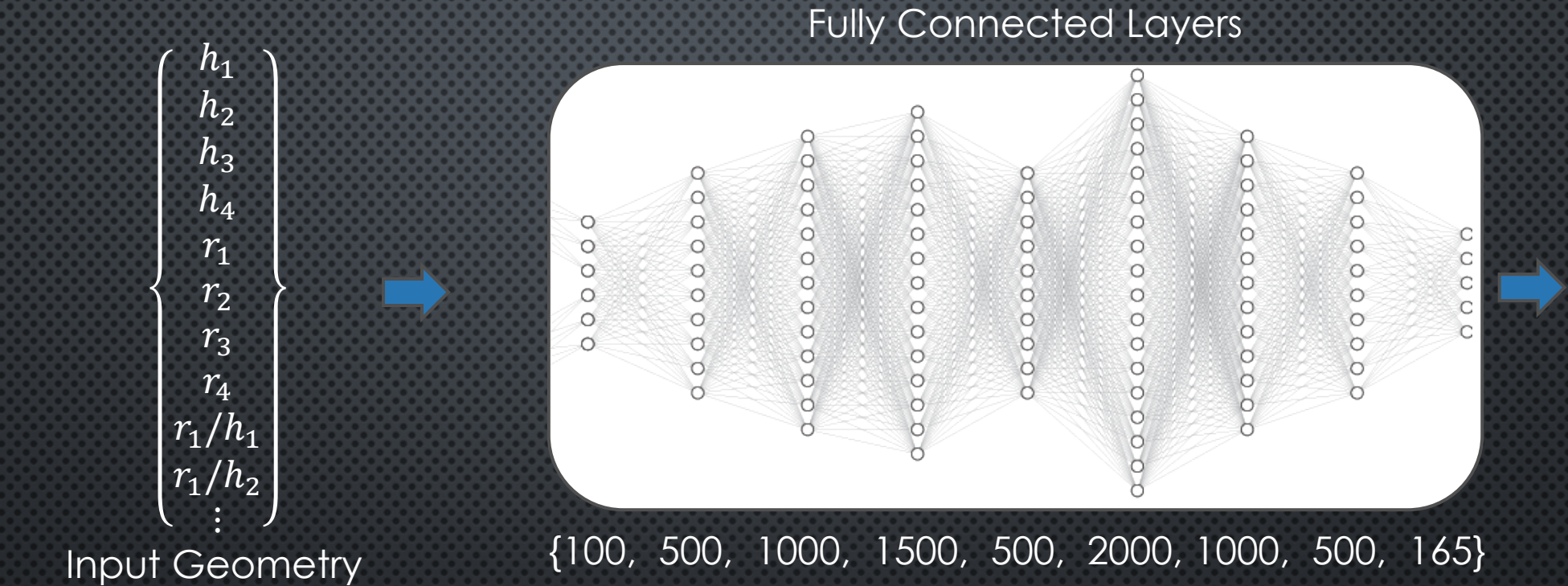


Predicted Spectra

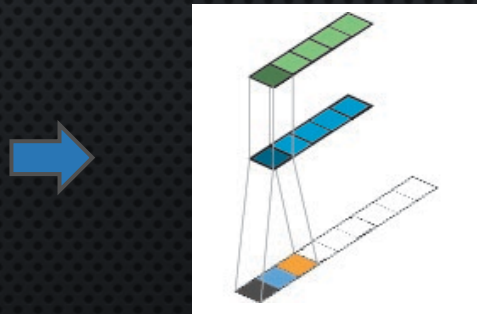




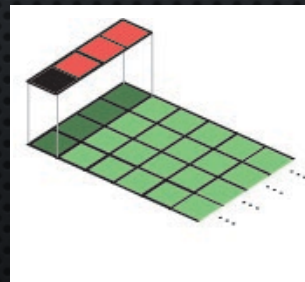
# NEURAL NETWORK ARCHITECTURE – RATIO INPUTS



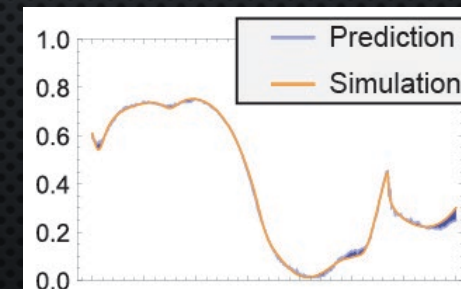
Transpose Convolution



Convolution

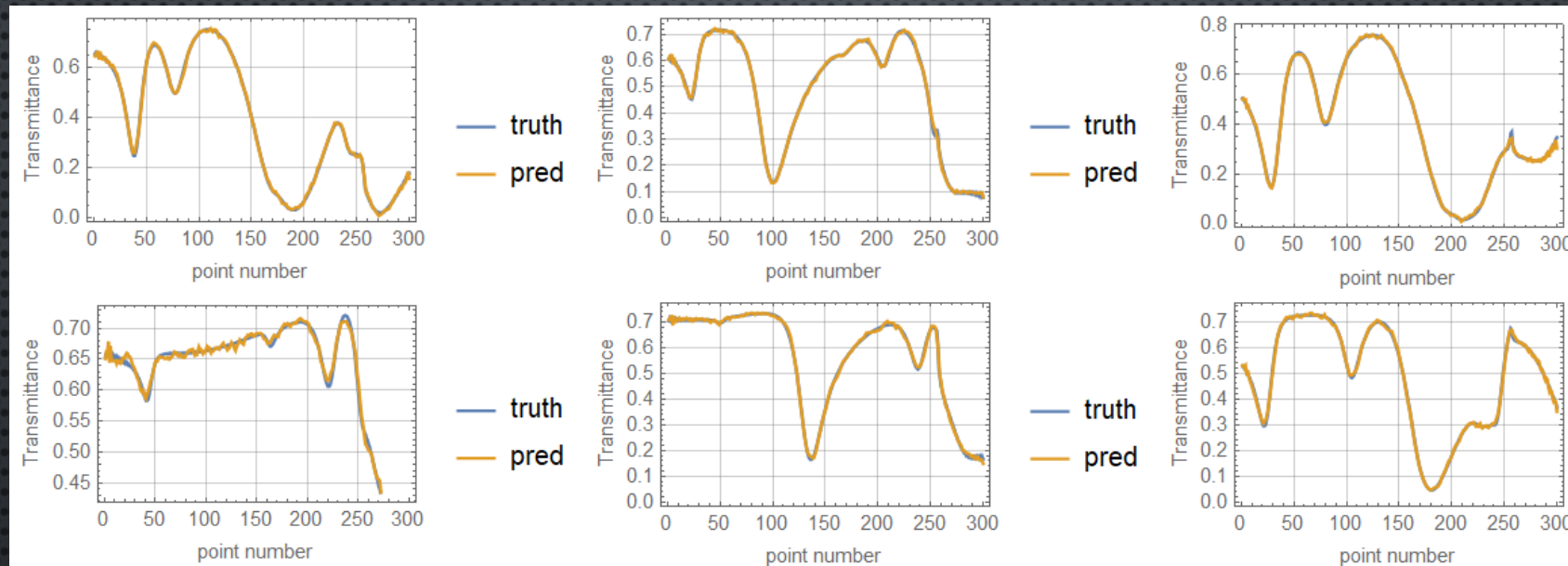


Predicted Spectra





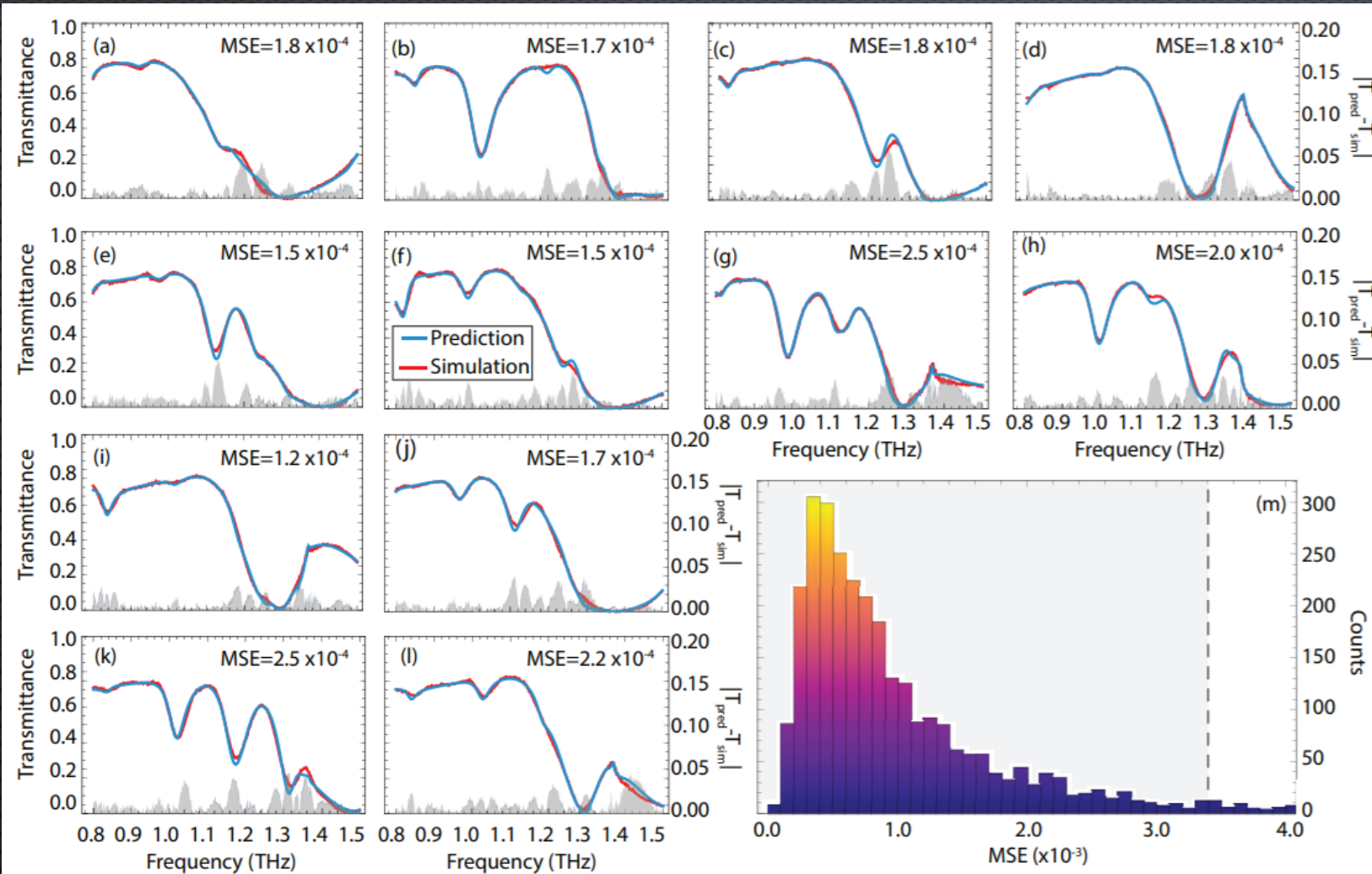
# MACHINE LEARNING RESULTS – NN ARCHITECTURES



1. Tensor module (TM)
2. Geometrical ratios (GR)
3. Neither TM or GR
4. Both TM and GR



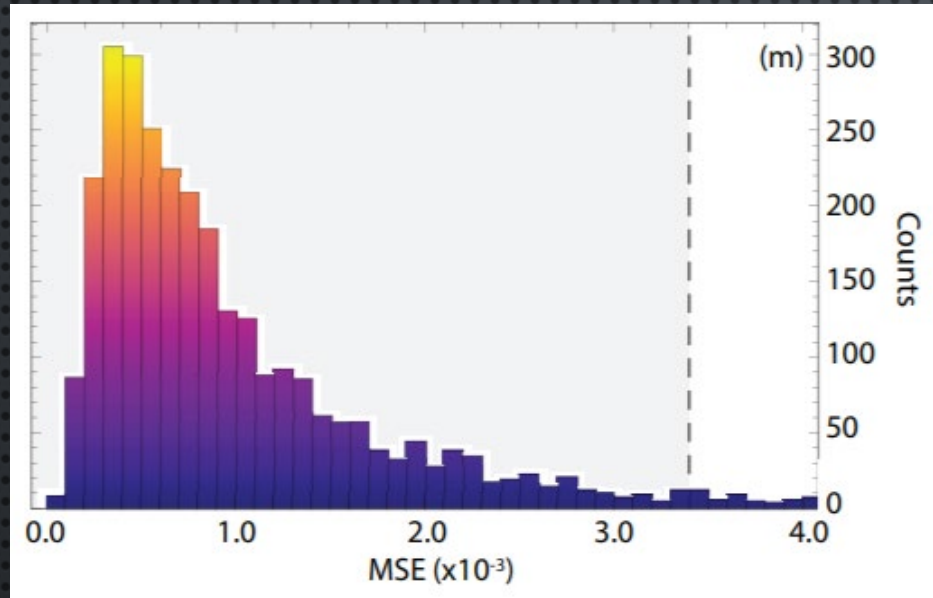
# MACHINE LEARNING RESULTS



- $MSE_{avg} = 1.16 \times 10^{-3}$
- 95% have  $MSE \leq 3.4 \times 10^{-3}$
- 99% have  $MSE \leq 6.2 \times 10^{-3}$
- Sampled only 0.0022% of the hyperparameter space



# PERFORMANCE OF MACHINE LEARNING ARCHITECTURES



<u>MSE</u>	<u>Tensor Module</u>	<u>Geometric Ratios</u>
$1.87 \times 10^{-3}$	yes	no
$1.41 \times 10^{-3}$	no	no
$1.32 \times 10^{-3}$	yes	yes
$1.24 \times 10^{-3}$	no	yes

## Tensor Module

$$r_i \times r_j \quad h_i \times h_j \quad r_i \times h_j$$

## Geometric Ratios

$$r_i/h_j$$

## Physics

$$\frac{r}{h} = 1.22 \frac{n}{\sqrt{n^2 - 1}}$$



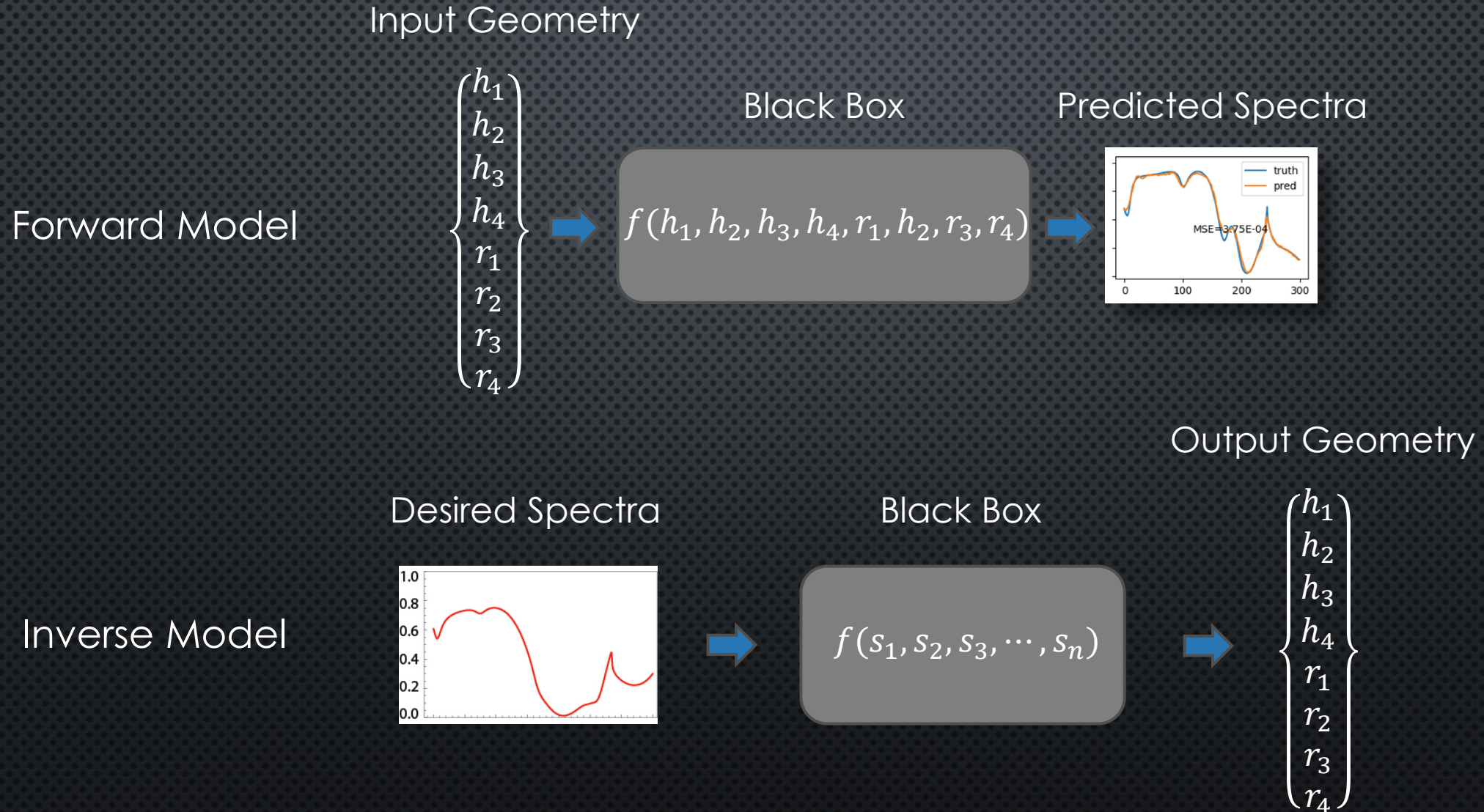
# OUTLINE

- ALL-DIELECTRIC METASURFACES
- MACHINE LEARNING
- **INVERSE DESIGN**
- ARTIFICIAL “INTELLIGENCE”
- CONCLUSIONS





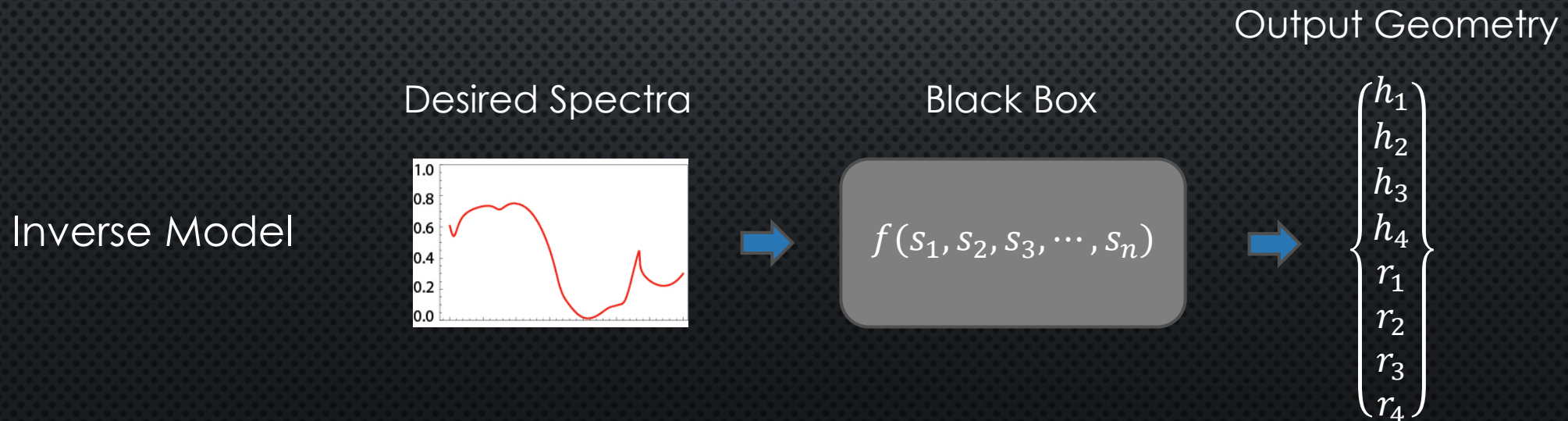
# THE INVERSE MODEL





# THE INVERSE MODEL

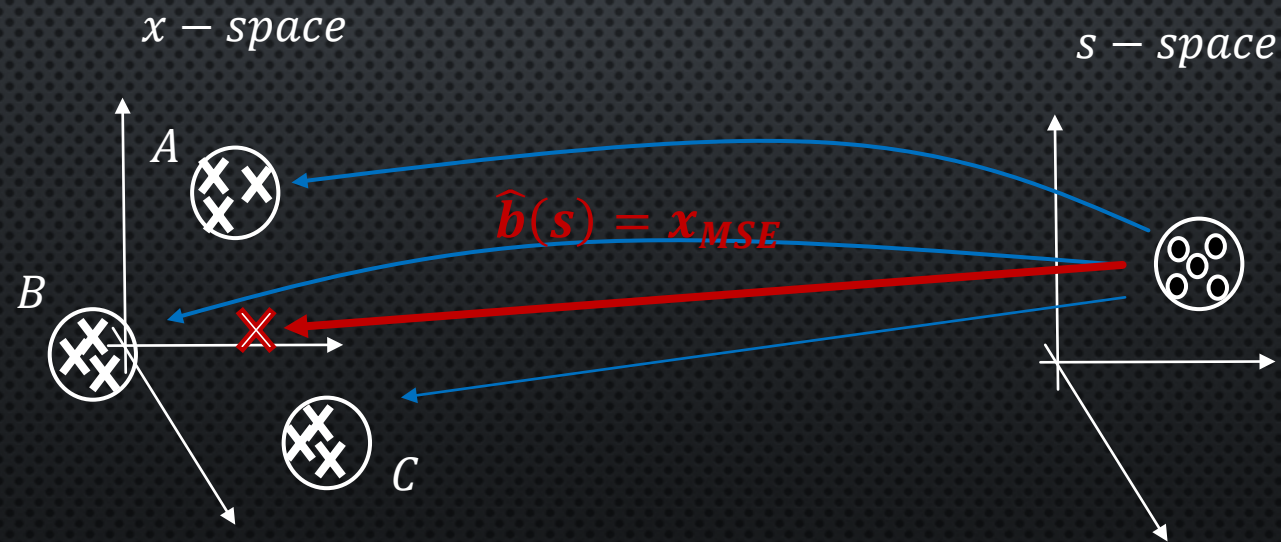
- There may be no geometry which realizes a desired spectra
- One-to-many mapping problem
- Does not indicate if a valid solution exists
- Does not provide a solution that *most closely* approximates desired spectra





# THE INVERSE MODEL

- There may be no geometry which realizes a desired spectra
- One-to-many mapping problem
- Does not indicate if a valid solution exists
- Does not provide a solution that *most closely* approximates desired spectra





# THE INVERSE MODEL

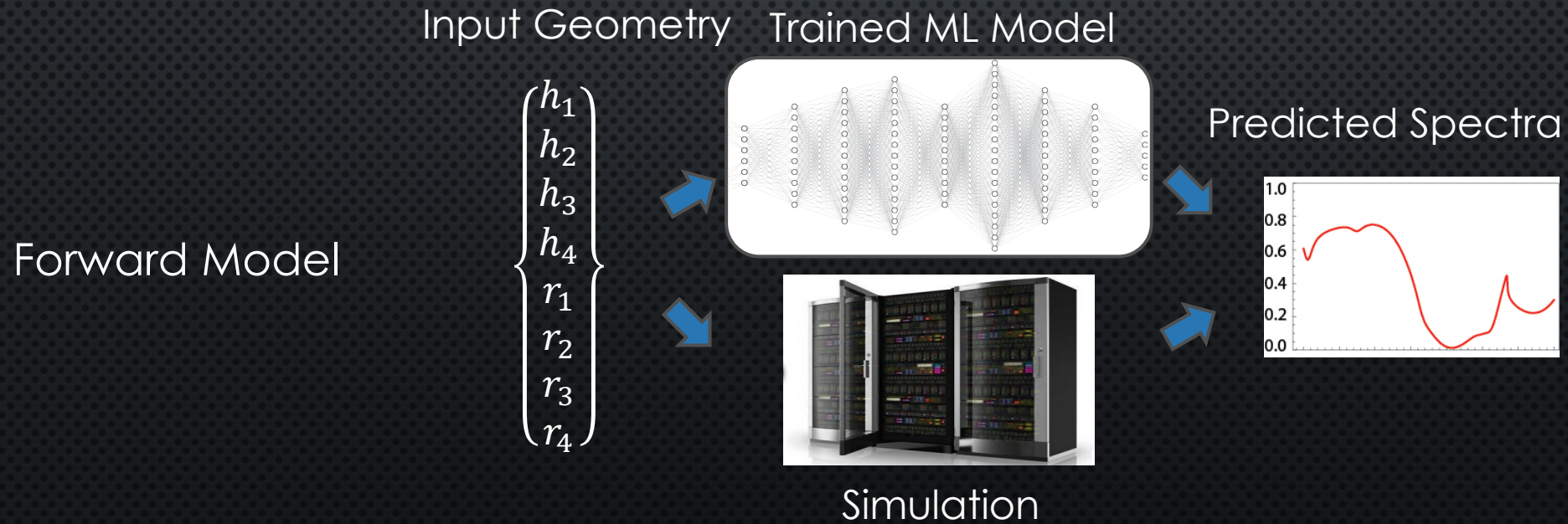


2200 years  
0.047 km/h

$\times 8.2 \times 10^5 =$



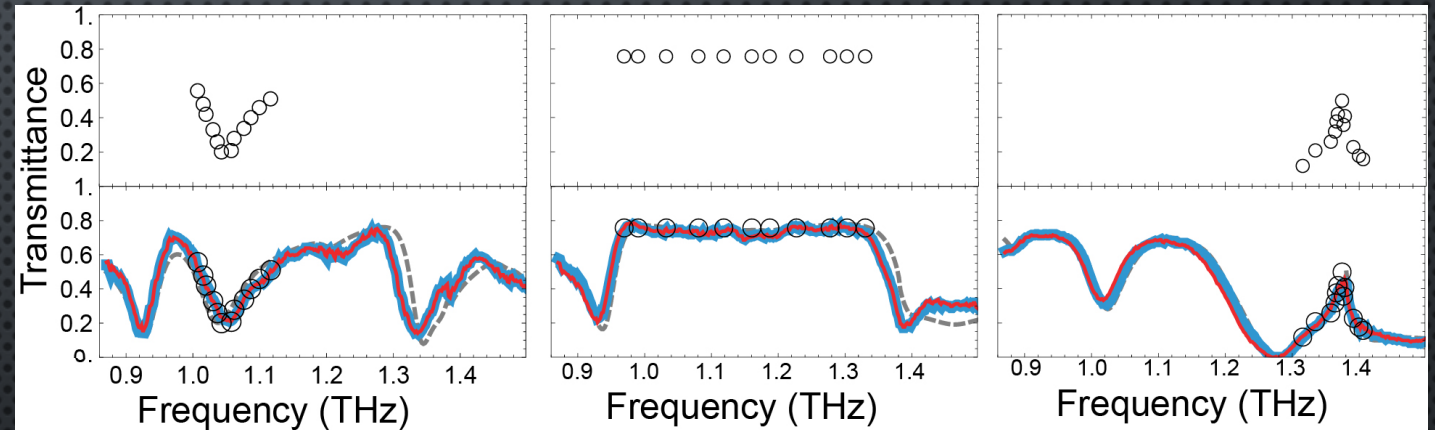
23 hours  
113 km/h





# FAST FORWARD DICTIONARY SEARCH

- $13^8$  total permutations  $\sim$  816 million
- 2200 years of compute time
- $8.2 \times 10^5$  faster than conventional solver
- ML calculates in 23h – 9900 sp/s
- 2.6 Terabytes
- Search rate = 40 Msp/s
  - $\sim$ 20 seconds for inverse solution



- Global optimal solution
- Second best solution
- Simulated global optimal sol



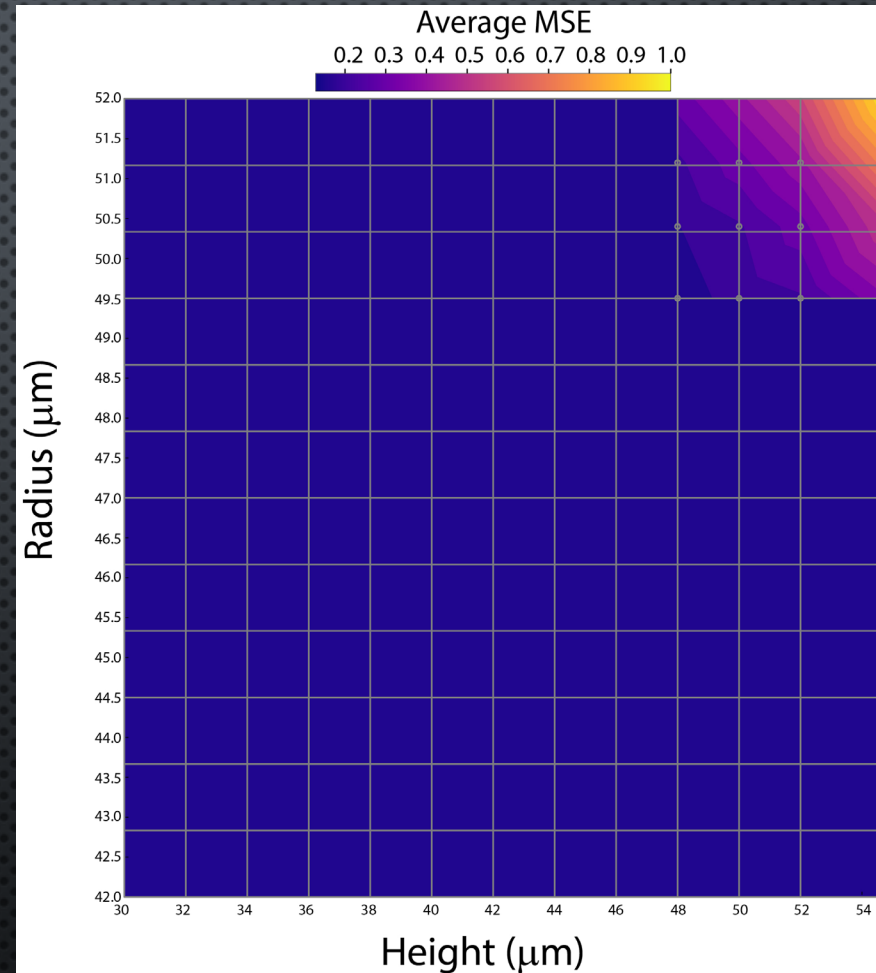
# OUTLINE

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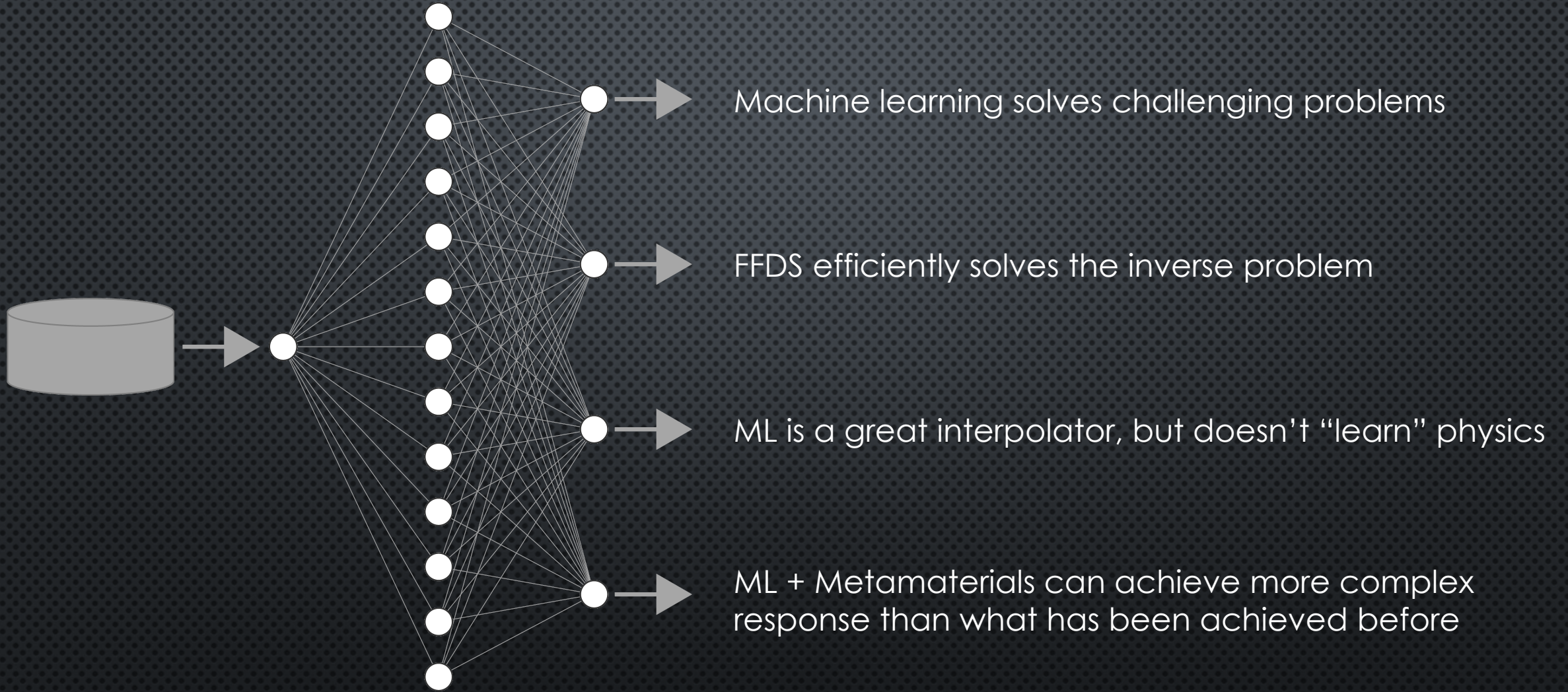


# DID THE NEURAL NETWORK 'LEARN' SOME PHYSICS?





# CONCLUSIONS





THANK YOU

