Using Computational Science to Address Key Challenges (from fundamental physics to real-world problems)

Two examples:

- Nano-medicine
- Materials by design

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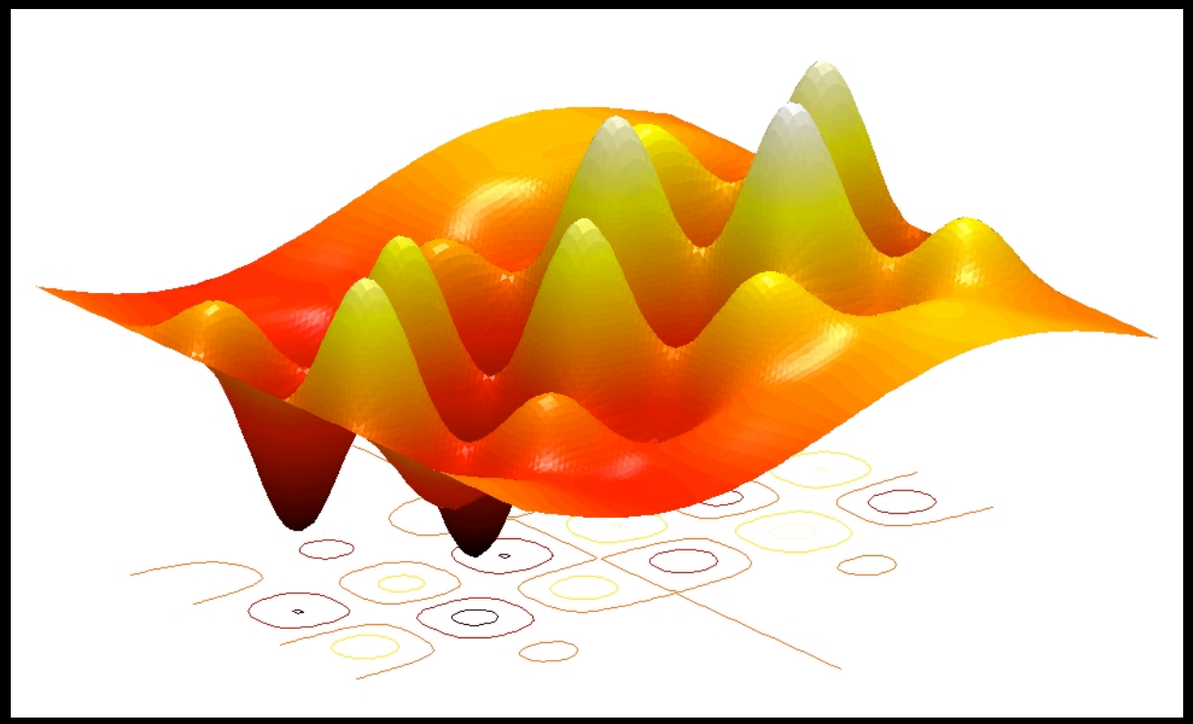
Physics & SEAS
December 02 2014

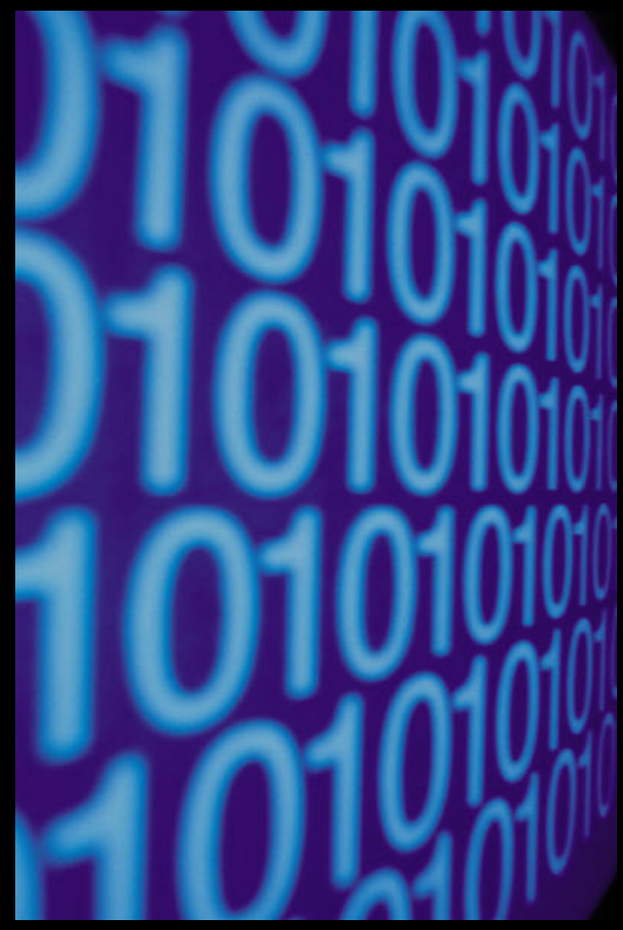
Computational Science



applied math

equations, theorems,
numerics, …

+



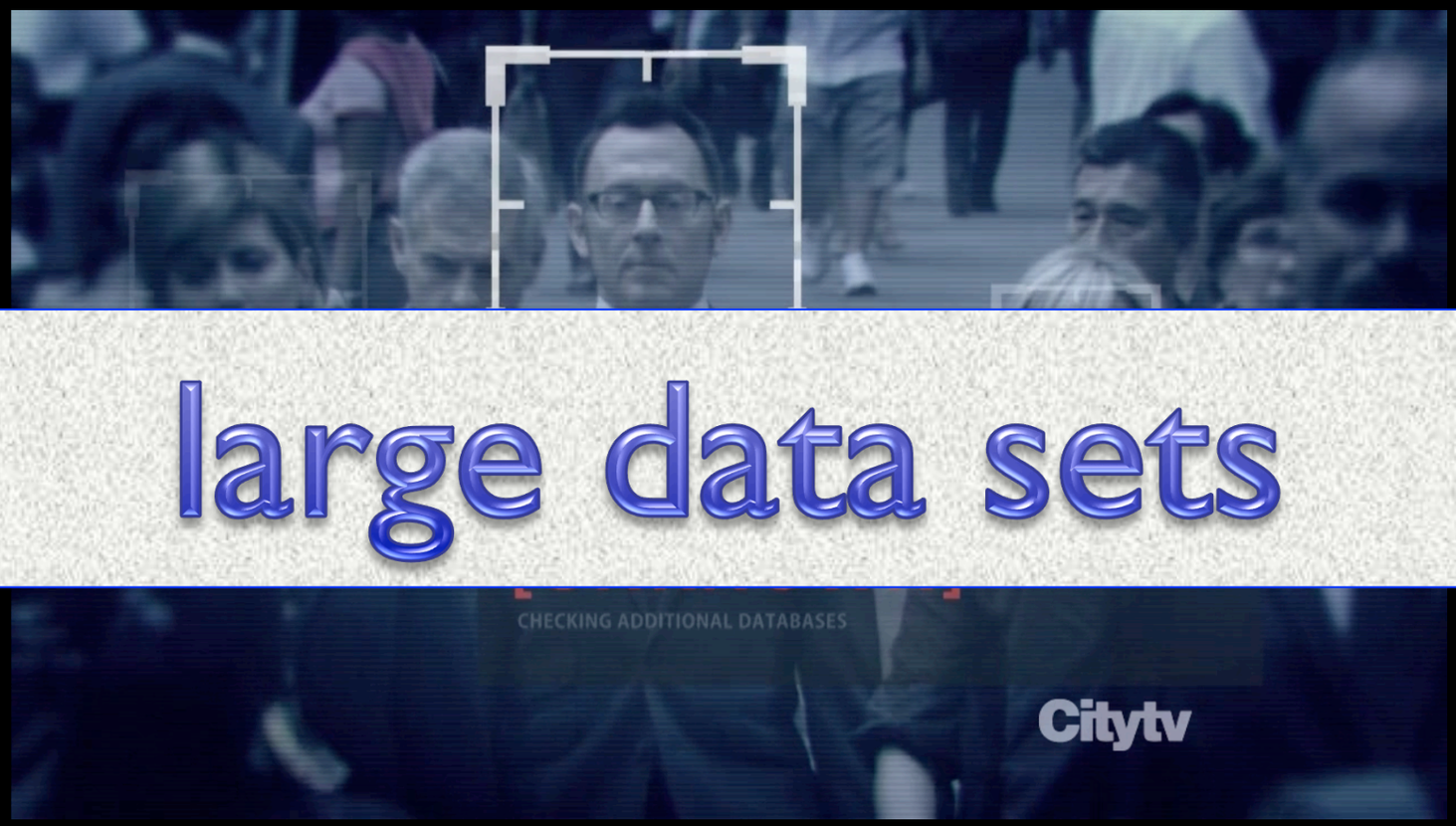
computer science

hardware, software, computing
algorithms, …

CSE is used to

- simulate
  - model
  - predict

complex systems



large data sets

- manage
- analyze
- visualize

Cardiovascular Disease

Leading cause of death in the western world

~1/3 deaths in the US alone

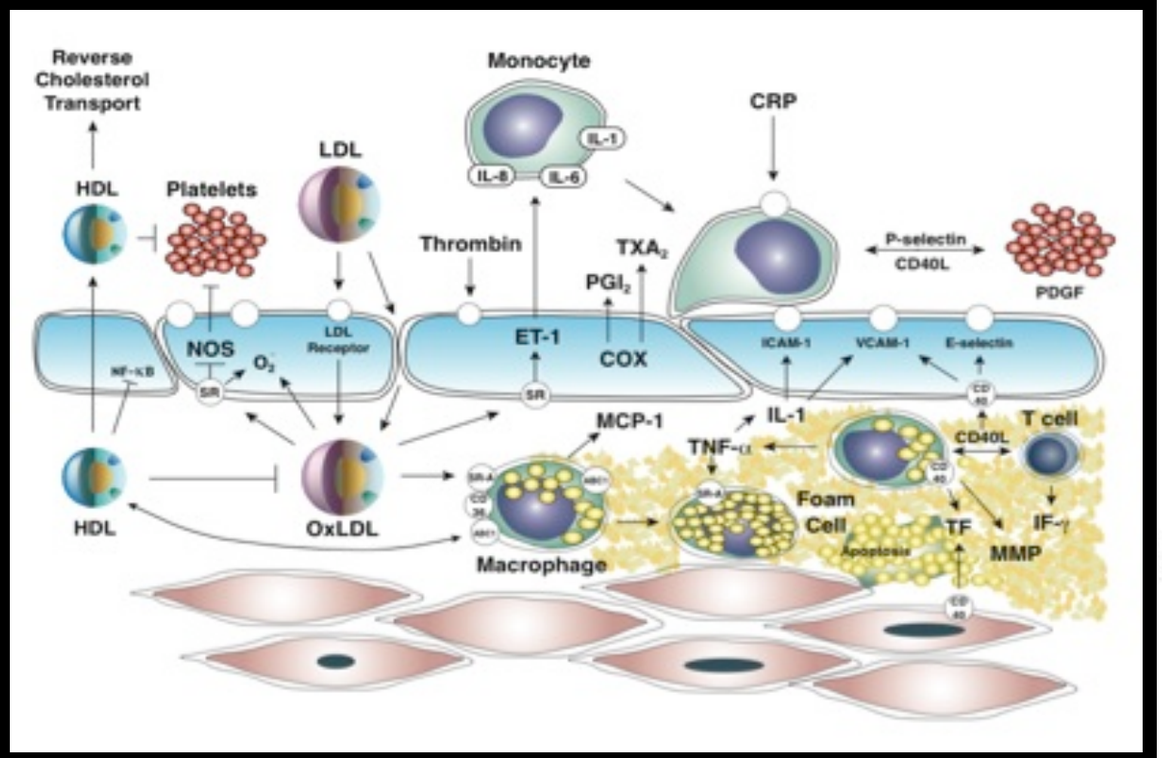
~50% of instances occur without prior symptoms

Komla Dumor was a highly acclaimed journalist who presented Focus on Africa on BBC World News, as well as being one of the lead presenters for World News' European morning segment.

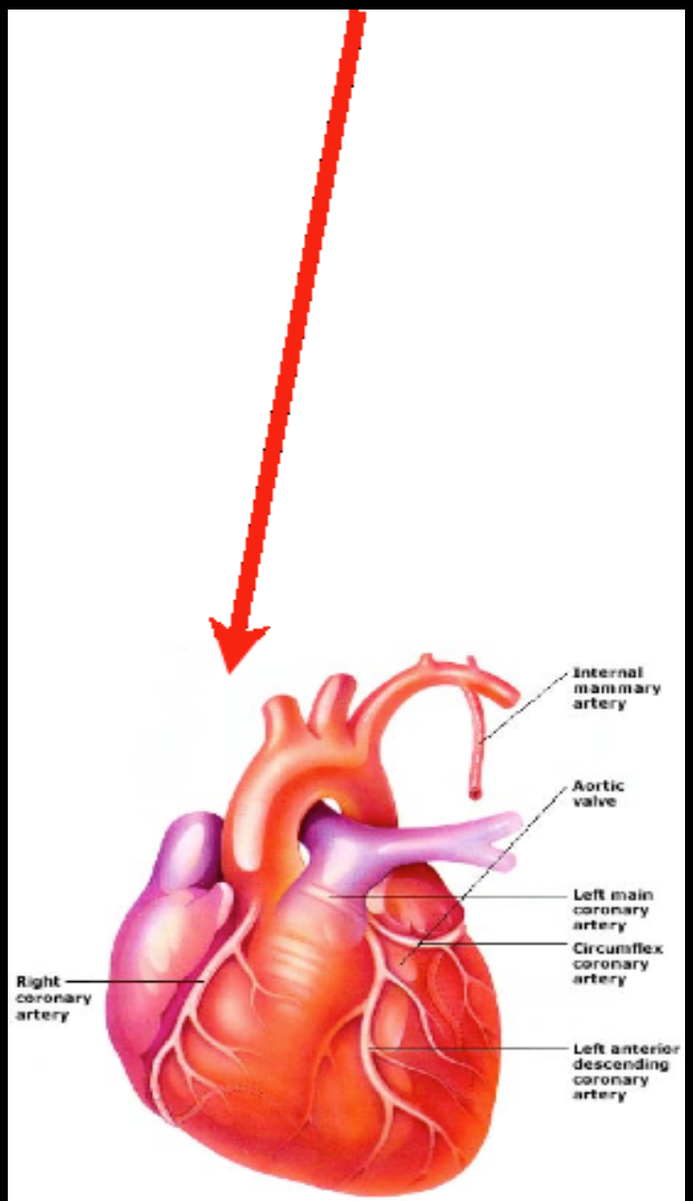
To the great shock and sadness of the BBC and its audience around the world, Komla died suddenly from heart attack in January 2014 at age 41.

Grand Challenge: Multiscale Hemodynamics

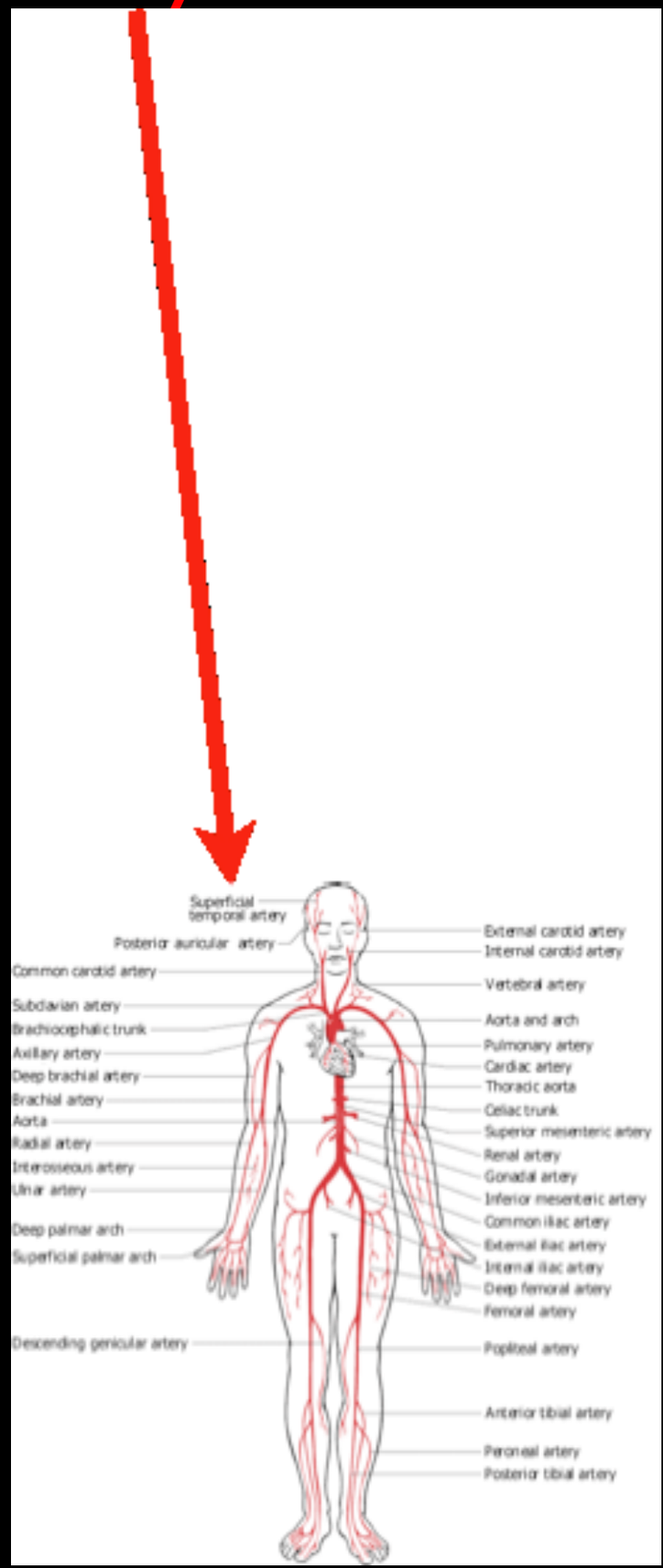
μm-nm scale – biochemistry



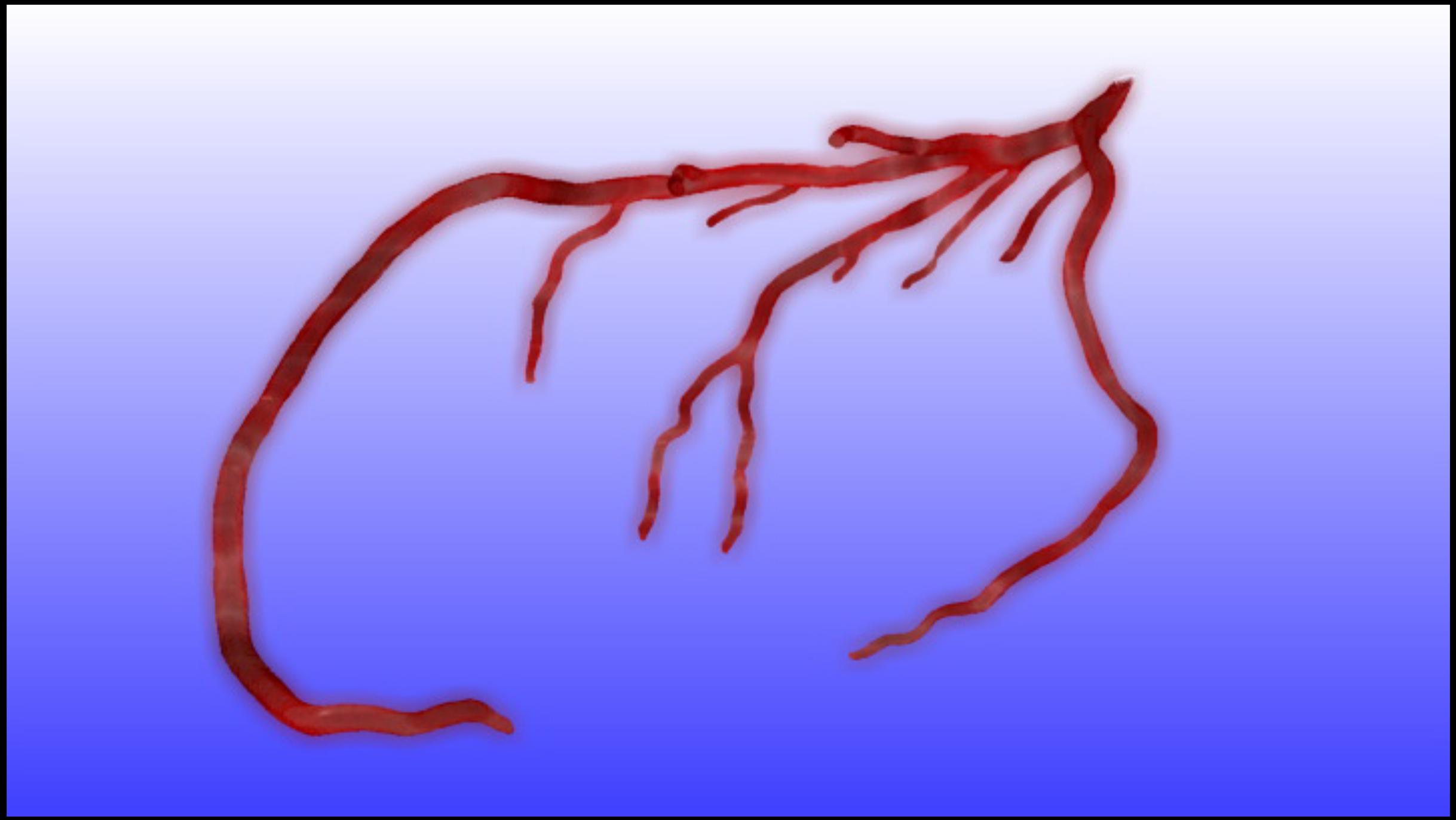
cm-mm scale – geometry/ fluid dynamics



m scale – boundary conditions

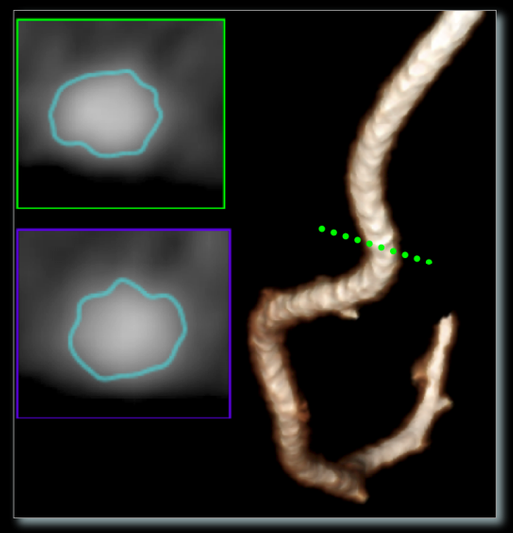


Full artery simulation: real patient data

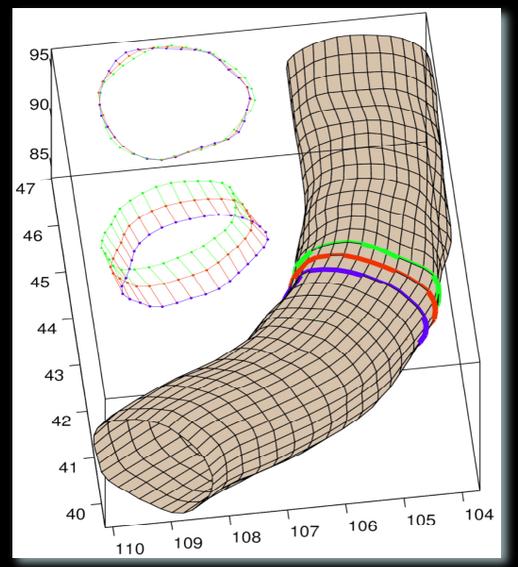


A. Peters, *et al.* Supercomputing, 2010

Patient Data



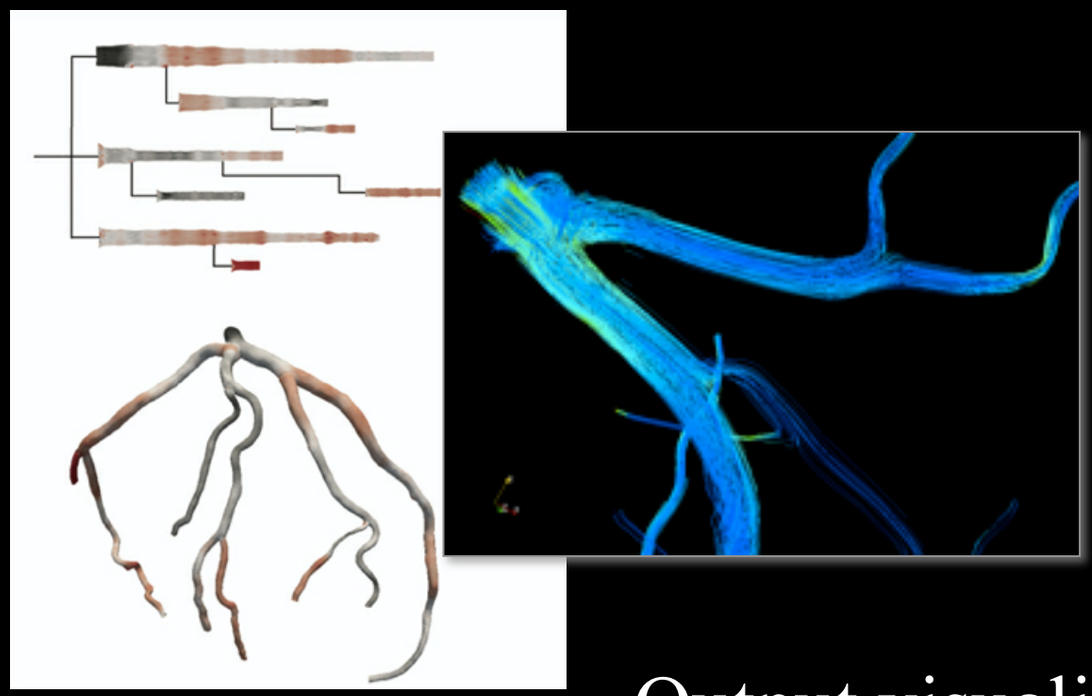
Data Segmentation



HPC Data Preparation

Parallel Code: MUPHY & HARVEY

Output visualization



Borkin et al. IEEE Transactions on Visualization and Computer Graphics, 2011

Materials: *Yesterday (cm - m)*

Locomotives

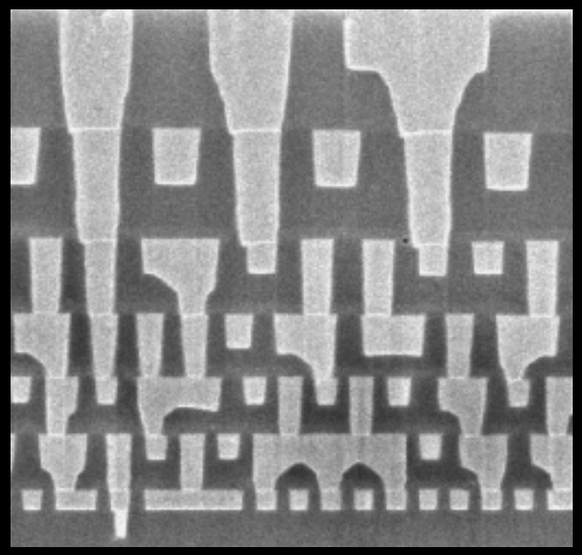
Automobiles

Bridges

Buildings

Materials: Today

Computing



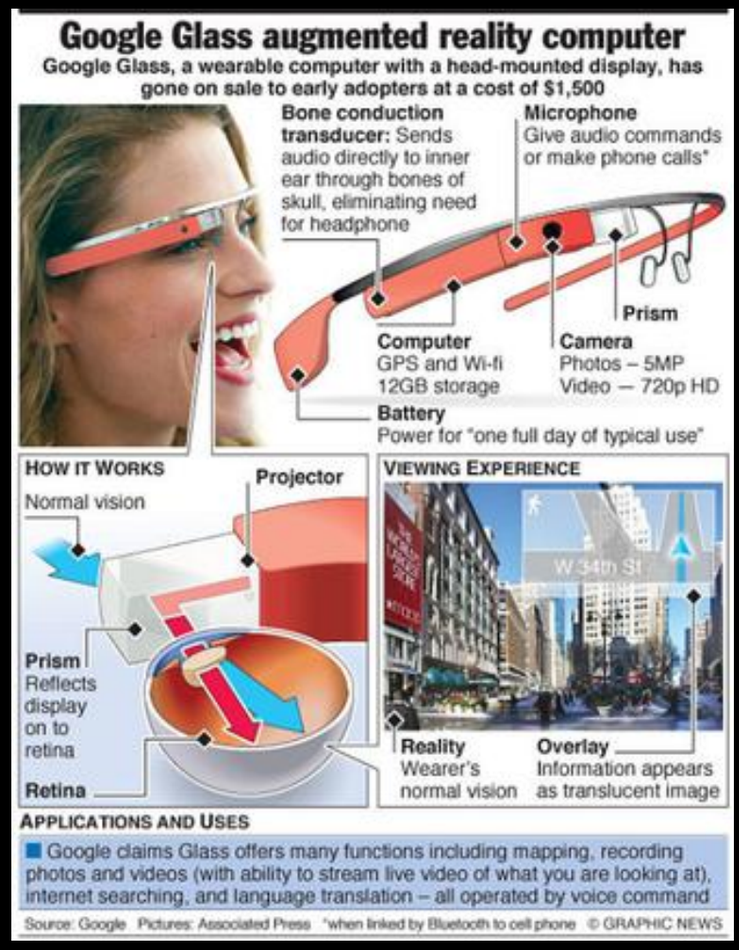
Transportation

- Unconventional materials used
  - Compound metal
  - Composite structure
  - Alkaline battery

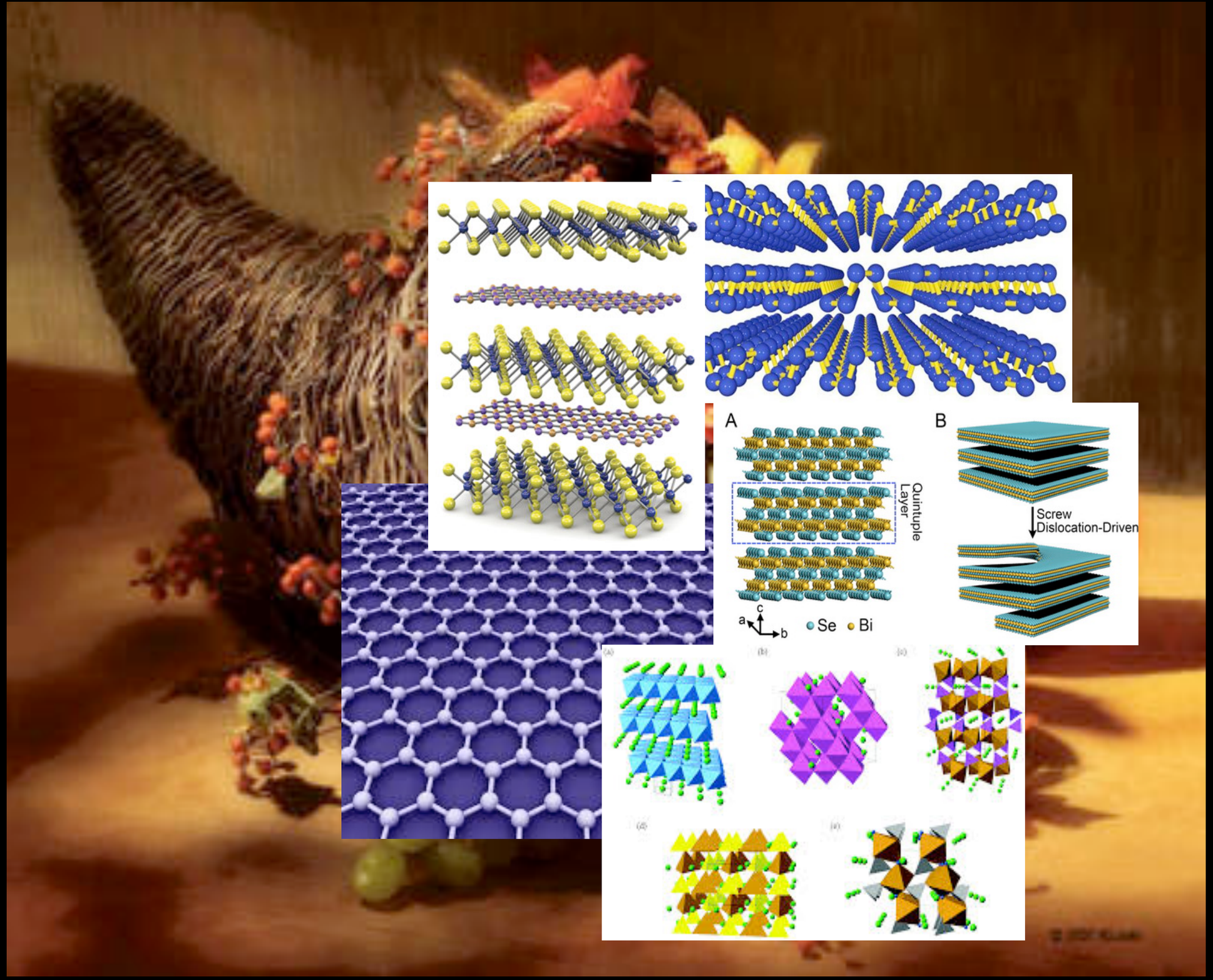
Materials: Tomorrow (nm)

Smart Phone

Smart Glass

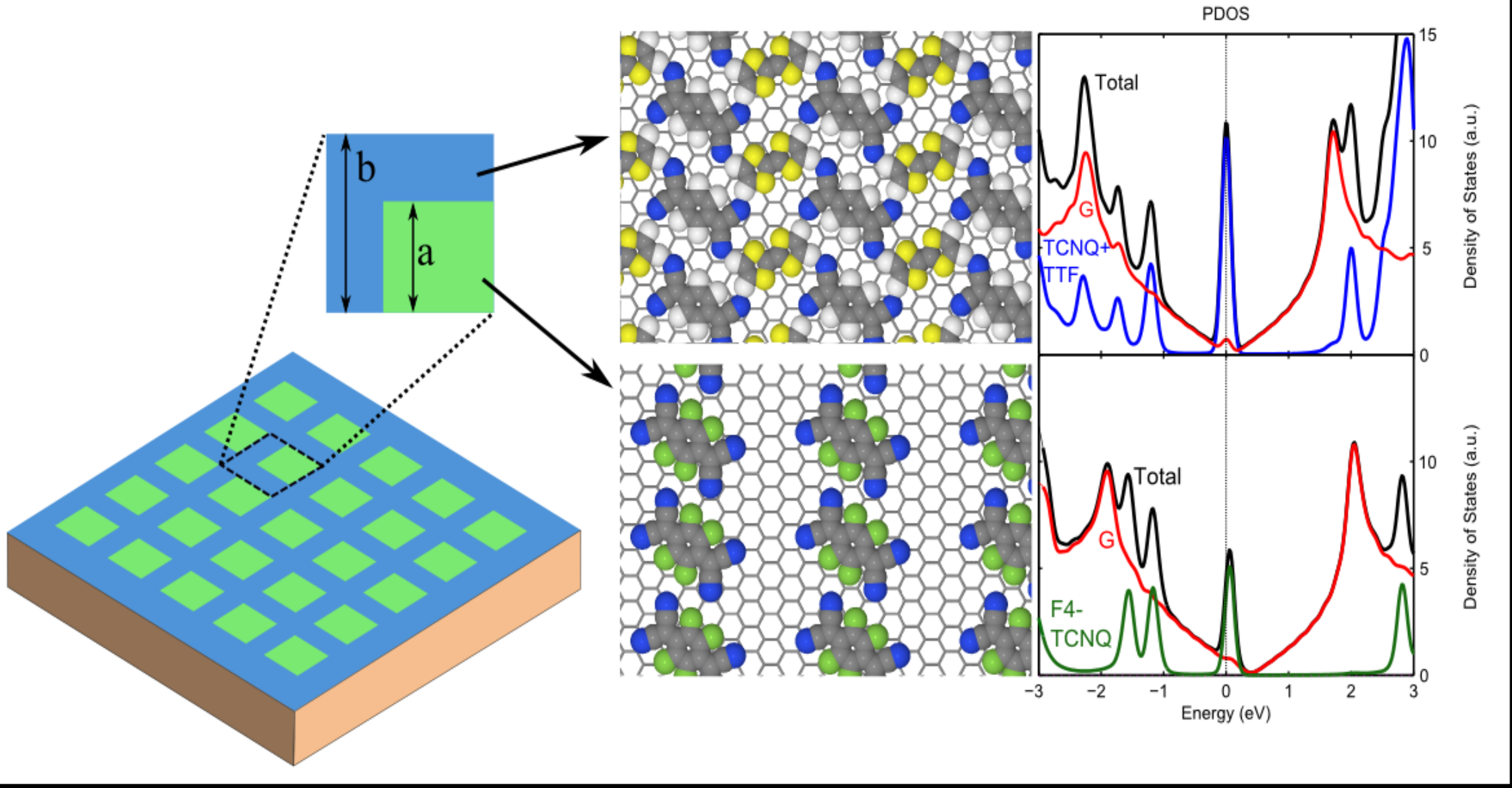


Properties and structures by design:
Materials Genome Initiative (Obama, 2013)



cornucopia (*cornu copiae*: Latin, "horn of plenty")
of new materials (2D): best way to combine them?

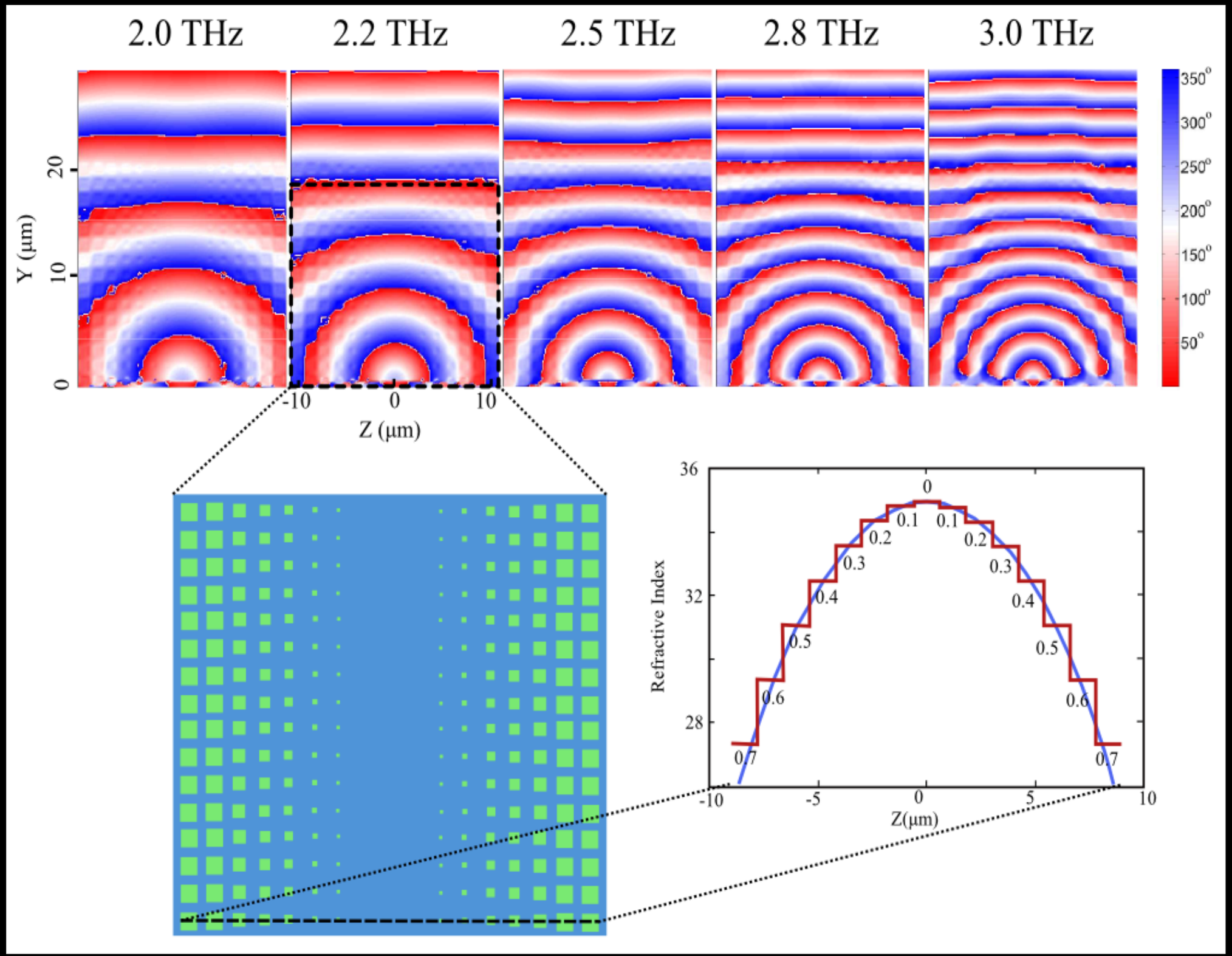
Proposed graphene-based plasmonic device



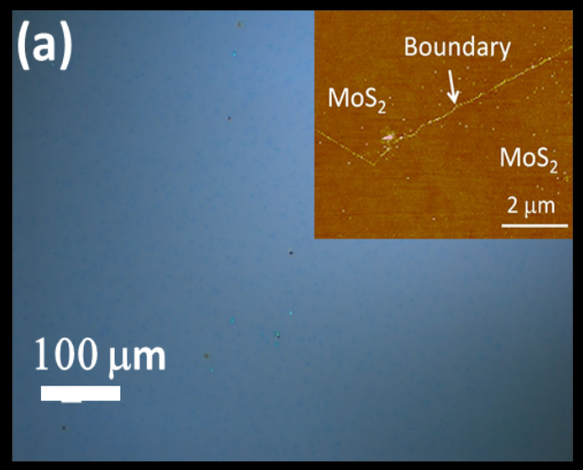
F4-TCNQ (blue area) and TCNQ+TTF (green area). Projected DOS shows effects of **doping** and the added molecular signature to the total DOS due to the molecule-graphene interactions.

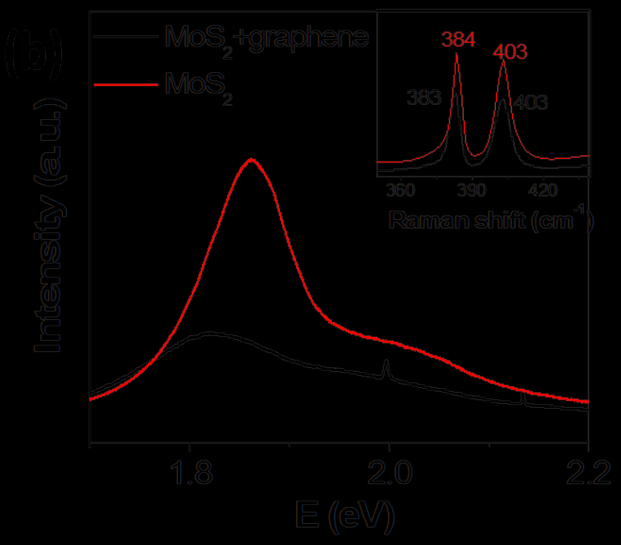
Selfoc lens: collimating EM waves

Jierong Cheng, Wei Li Wang, H.M., E.K. NanoLetters 2013

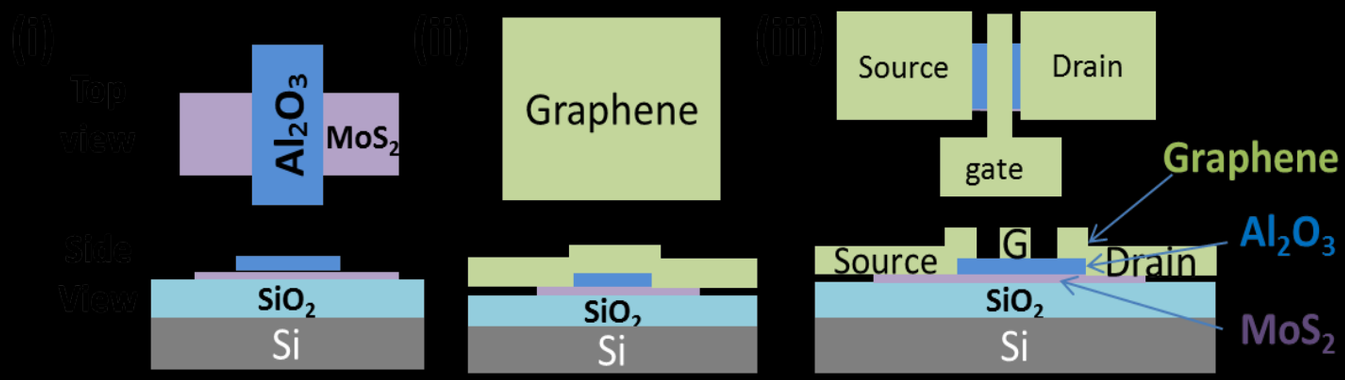


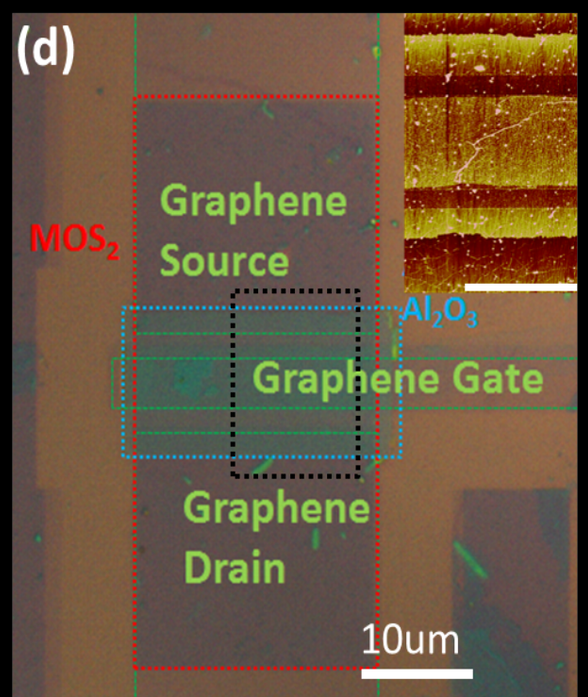
MoS_2-based Electronics: barriers to contacts

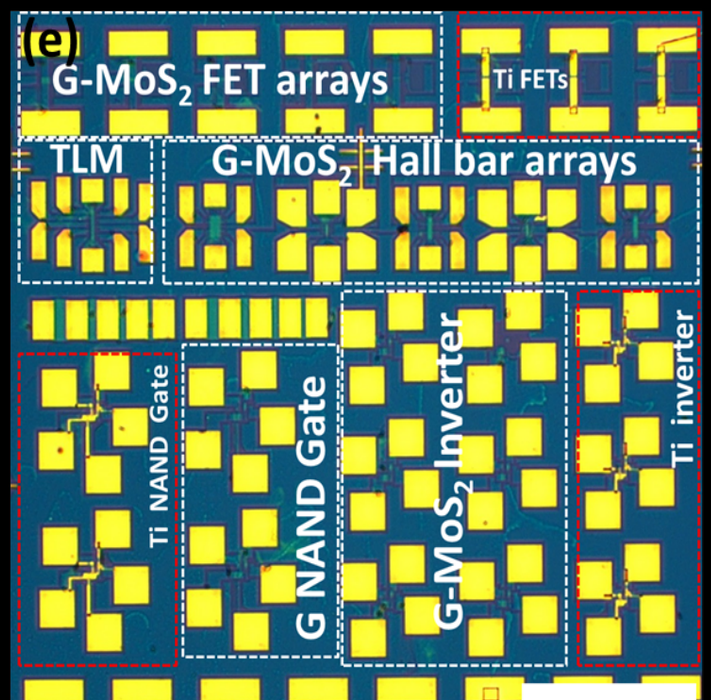




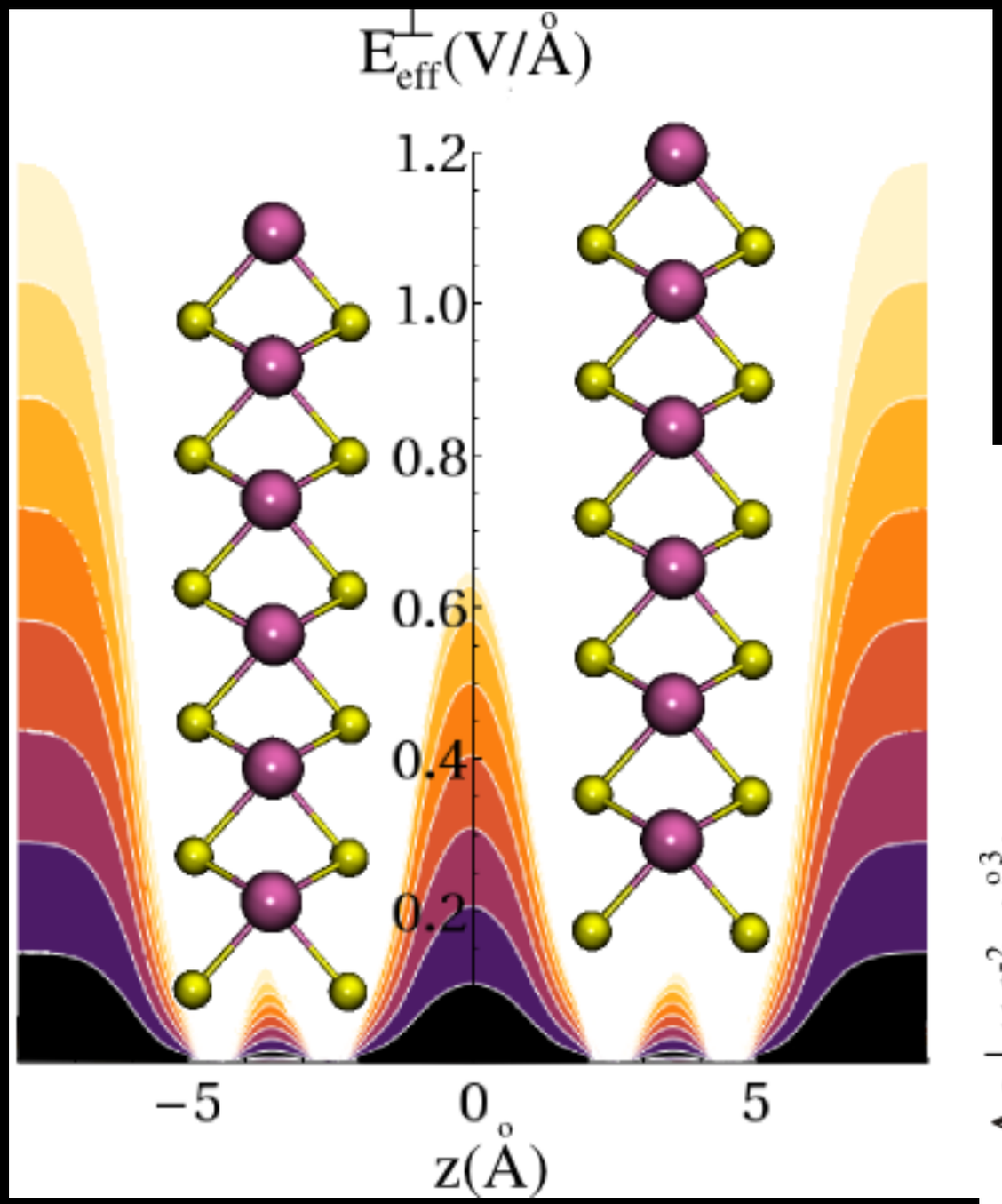
Tomas Palacios group (MIT)
Lili Yu *et al.*, NanoLetters 2014



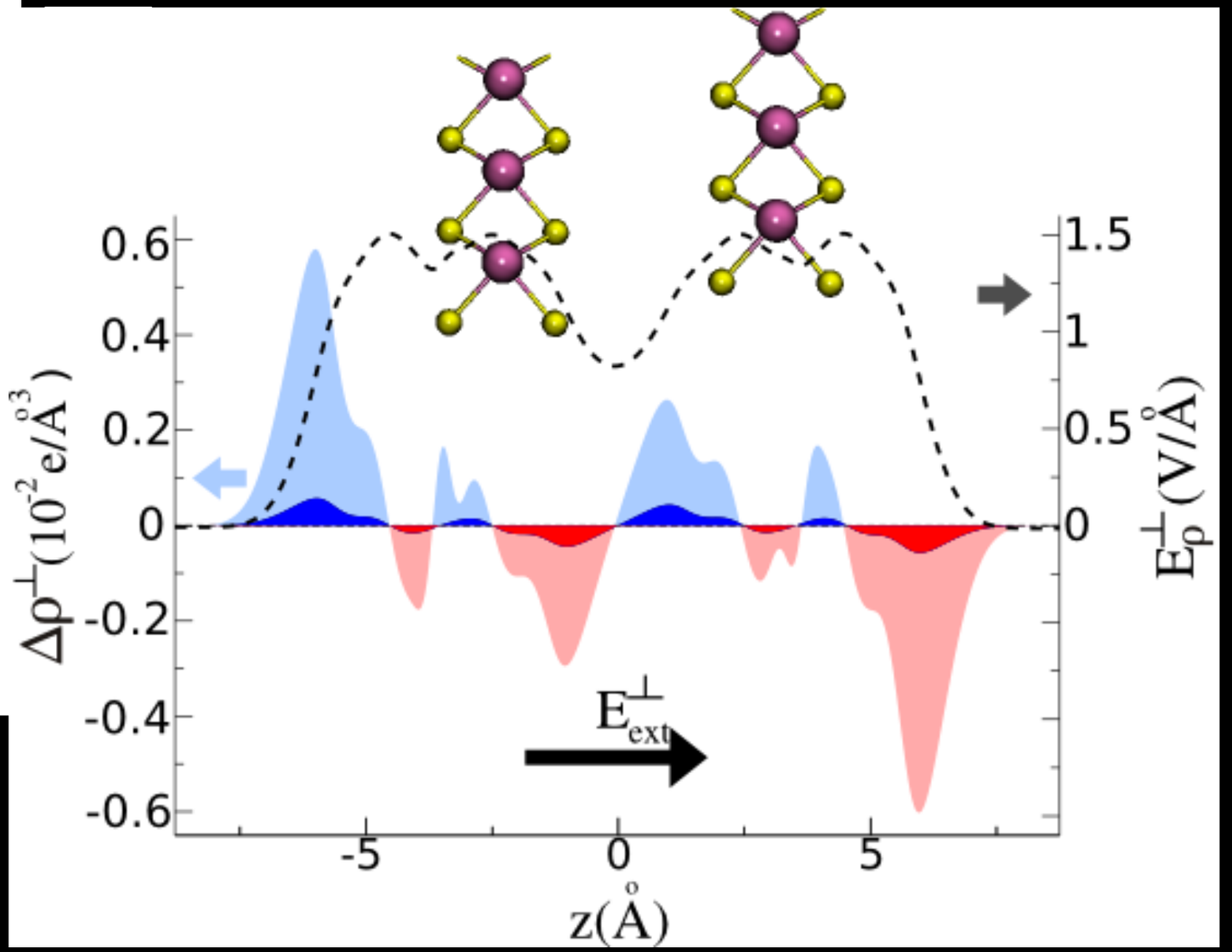




Shielding effects due to polarizability of MoS_2 layer



The polarization charge and
the response field
depend on external field



The country that
out-*computes*
will be the one that
out-*competes*.

U.S. Council on Competitiveness, 2004