Application Technology Team for *Nanomaterials*

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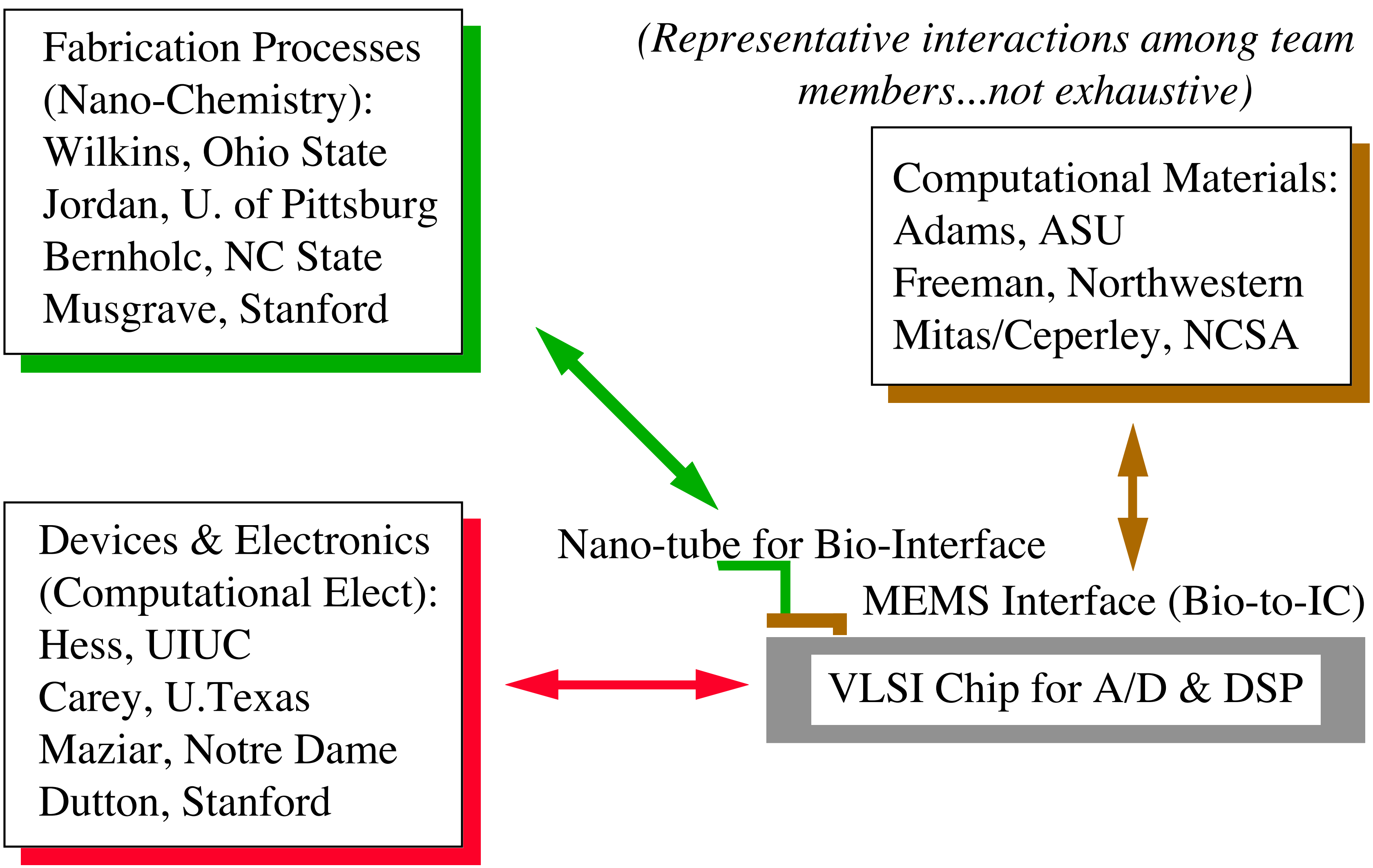
http://www-tcad.stanford.edu/

- 21st Century Technologies can be built atom-by-atom
- This thrust seeks to build the necessary analysis/design capabilities and supporting science to achieve computational nanomaterials
- Driver Technologies:
  - ***Micro-electronics***
  - ***Bio-****materials/Bio-sciences*
  - ***Micro-/Nano-mechanics***
- Representative examples and cross-links among the Alliance team in the Nanomaterials AT are now given

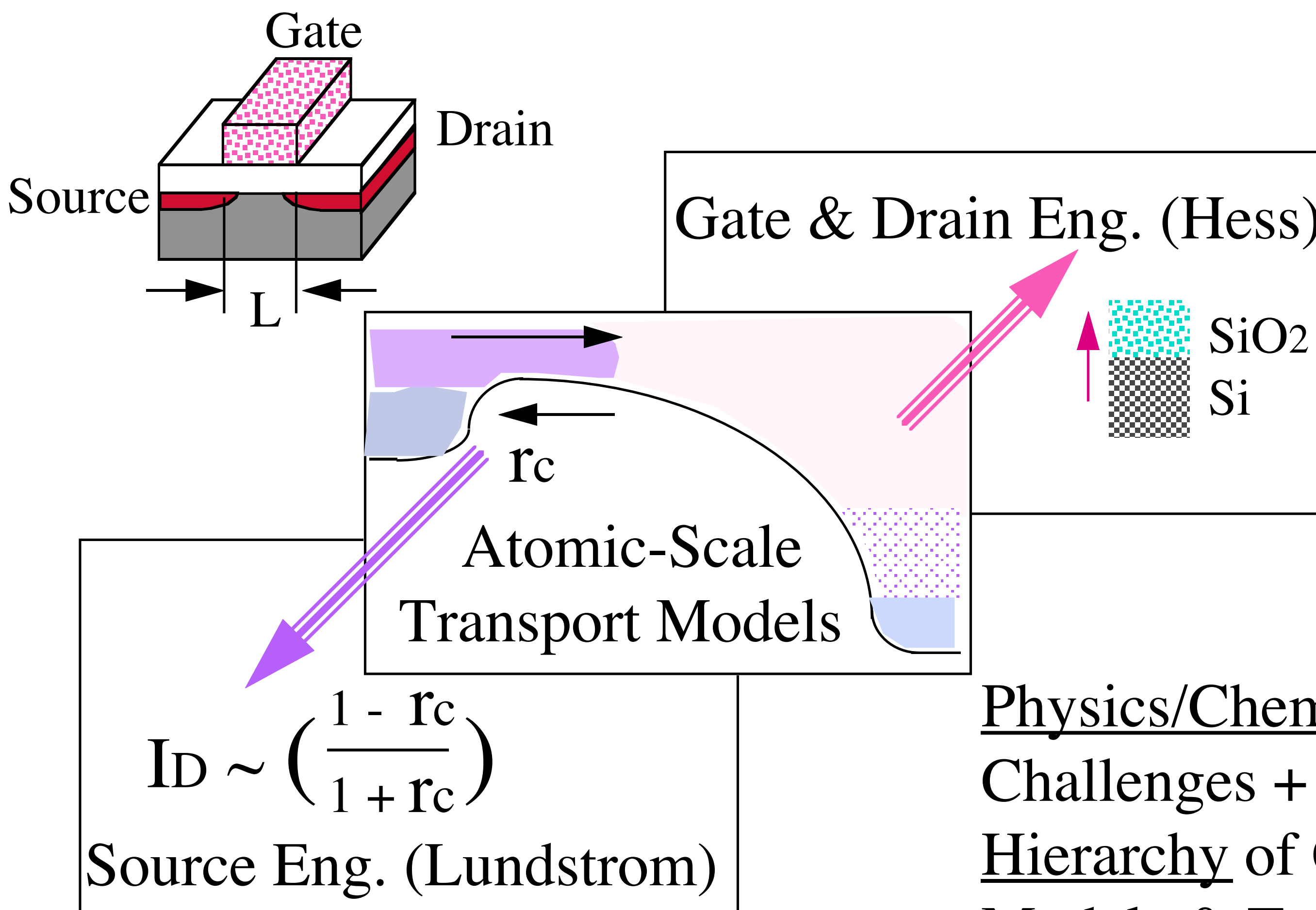
Fabrication of Nano-Structures

(A scenario of a 21stC “chip” with Composite Technology integration)



Example from Computational Electronics

*(Nat'l Center for Comp. Elect.--**NCCE**)*

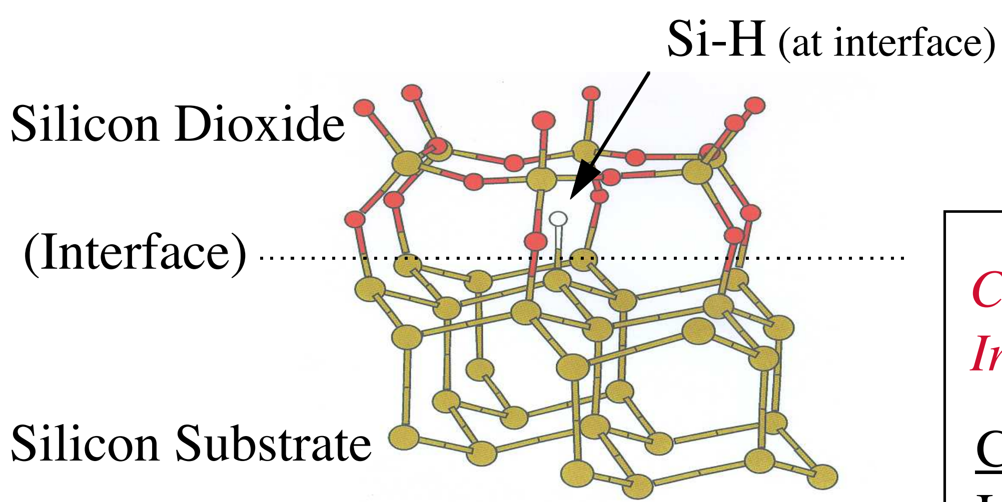


(Users: SRC, **NNUN**...)

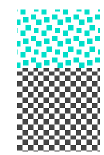
<u>Physics/Chemistry/Materials</u> Challenges +
<u>Hierarchy</u> of Computational Models & Tools +
<u>Engineering Methodology</u> to Use in Real Applications

Atomic-Scale Modeling of Interfaces

(Hess, Register, Tuttle, Lyding --Beckman/UIUC)



Closer Look at Interface Physics

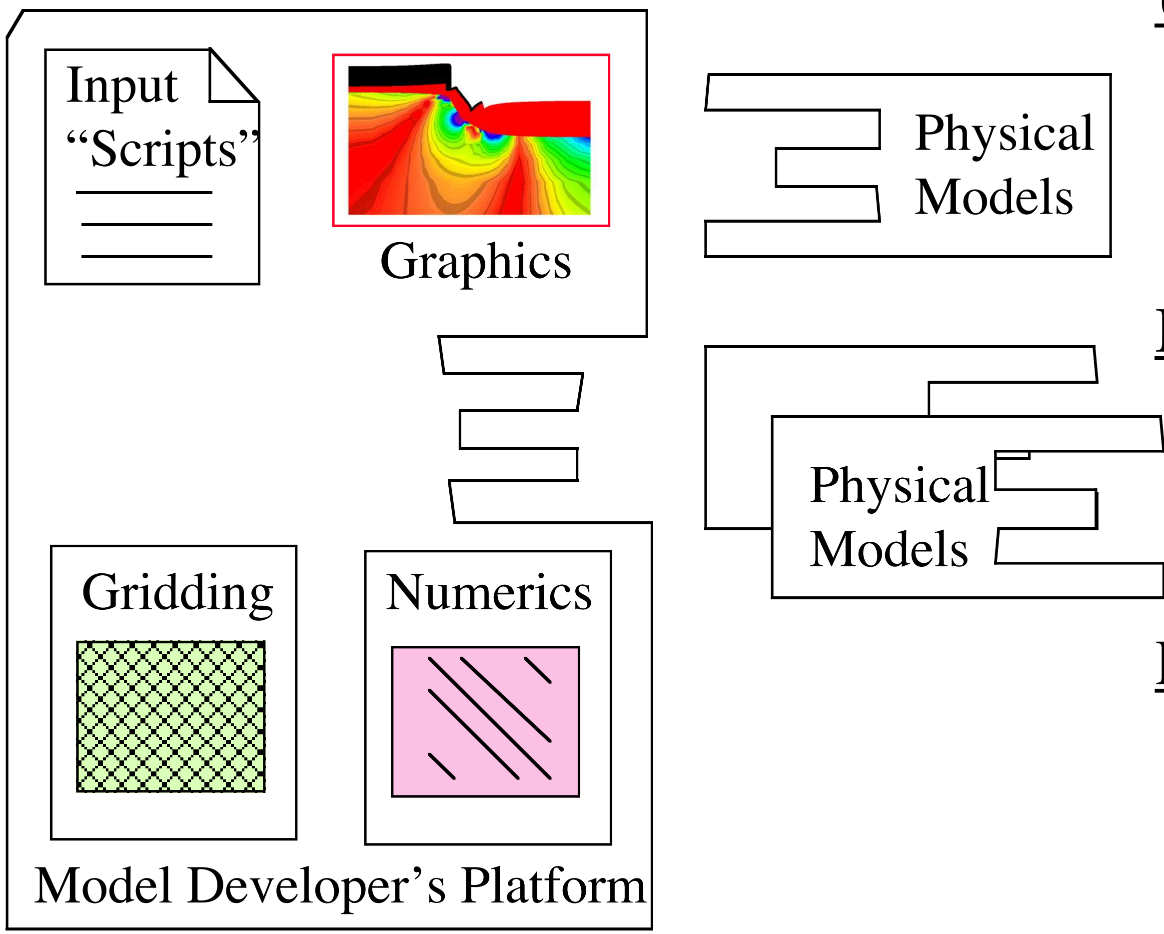


<u>Computational Model of Interface Scaling in CMOS</u>

- Ab-initio (and QM) of Si-H energetics
- Influence of hot carrier transport (MC or PDE)
- Process innovations based on surface chem.

PDE-based Hierarchical Modeling

(Dutton-Stanford, Carey-UT, Lundstrom-Purdue…NCCE)



<u>User Level:</u>
- Portable Scripts
- Benchmarks
- Applications

<u>Model Developer Level:</u>
- Physics
- Coupled Systems
- Materials DB

<u>Platform Developer Level:</u>
- Performance
- Libraries
- User Access:
  - GUI
  - Internet…

Summary & Conclusions

- Nanomaterials AT seeks to capture and use **atomic-scale** information across composite (heterogenous) technology/application domains
- Interdisciplinary teams cross-link areas of both **science and engineering**
- Example from future **IC-based Nano-Fab** shows:
  - interactions *(Chemistry, Materials, Devices...)*
  - need for atomics *(which also drives computations)*
  - leverage in creating more flexible *(and powerful)* Developer's Environment (visit our web site and look at PROPHET... http://www-tcad.stanford.edu/tcad/NCSA/)