Slide 1

## Theoretical Investigations and Simulations of Nanotube Properties

V. Meunier
Materials Science Group
Computer Science and Mathematics Division

Namur University, Belgium (1996-1999)
NC State University (2000-2001)



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## Strength and expertise at ORNL

- Renowned expertise in nanotube research
  - Intercalation
  - Composites
  - Doping & defects
- Close collaboration with experiments
  - Simulation and interpretation
  - Aid in guiding experiments
- Large scale computational methods
  - Scaleable and massively parallel programming
- Center for Computational Sciences
  - Materials focus area
  - World class resources



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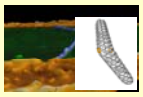
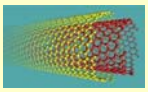
## Conventional nanotube materials

*SWNTS*

*SWNTS ROPE*



*Intramolecular junctions*



*MWNTS*

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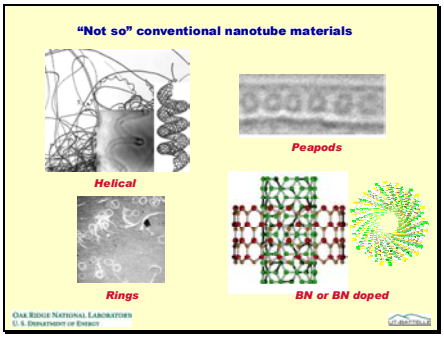


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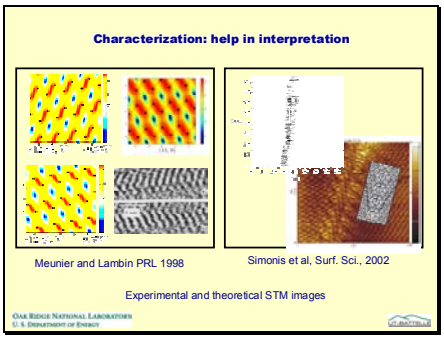


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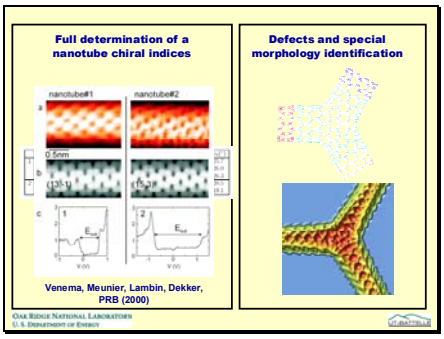

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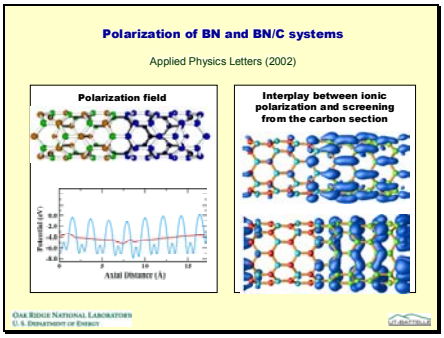


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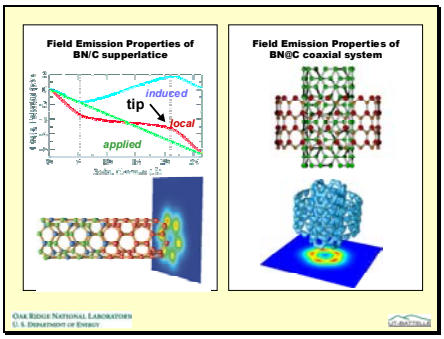


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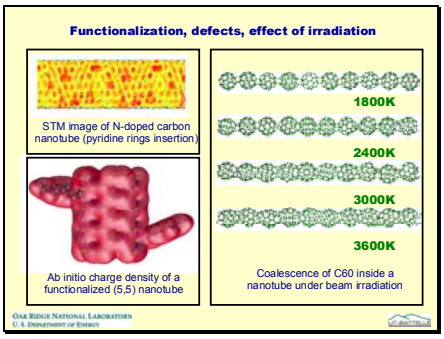

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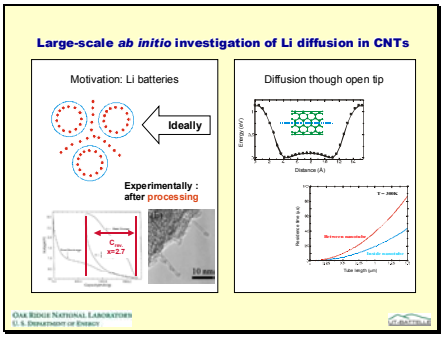


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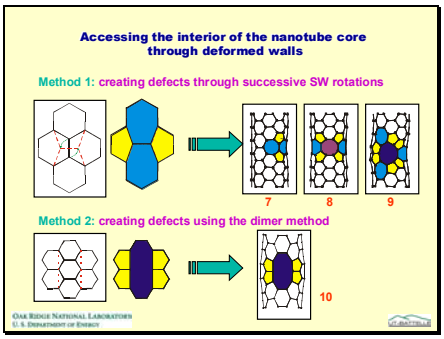


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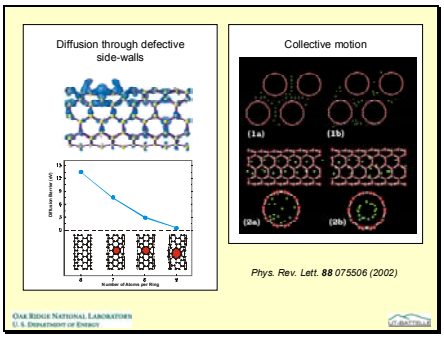

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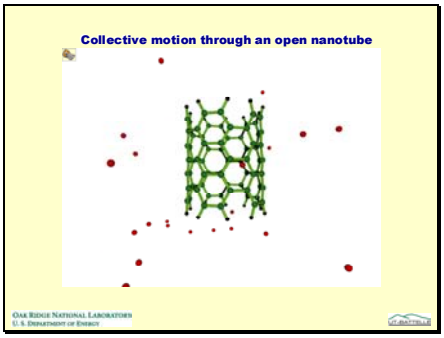


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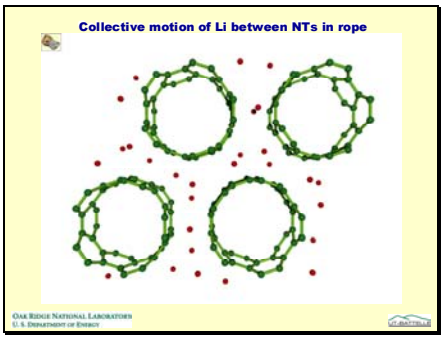


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