Computational Materials Science
Theme 3:
Fostering Science-based Discovery/Optimization of Novel Multifunctional Materials through Computational Materials Science
CMS at different “scales”

- If more than one “box” is involved in a computation → multi-scale modeling

Enablers:
Advances in:

- Theory
- Methods
- Software and Hardware Infrastructure

e.g., density functional theory (DFT)
Where are we now?

- **Theory:** Acceptable Level of Maturity
- **Methods:** Significant advances in past decade
- **Infrastructure:**
  - Less than a decade ago:
    - Impossible even to think about computer-aided materials design
    - To keep things in perspective:
      - Computing power has increased by two orders of magnitude in 10 years!
      - Will increase by another three in less than ten years
  - **Exascale computing**

wikipedia
Multi-scale Materials Modeling: Two Paradigms

- **Concurrent Modeling:**

- **Hierarchical Approaches:**
Computational Materials Science: How is it used?

• CMS enables:
  – Explain phenomena beyond experimental resolution
  – Discover new unexpected phenomena
  – Predict properties
  – Design new materials

• Constrains experimental search space
(General) Challenges:

- Concurrent or hierarchical modeling?
- How to exchange information between scales?
- What to do when phenomena at multiple scales are tightly coupled (parameter-passing not sufficient)
- How to decide what to ignore?
- Bottom-up, or top-down?
• (IIMEC) Challenges:

– How can we use CMS effectively within IIMEC collaboration?
– Can we take grand challenges from our experimental colleagues?
– What methods and techniques do we have?
– What capabilities are yet to be developed?