PHYSICS-BASED MATHEMATICAL MODELS OF LOW-DIMENSIONAL SEMICONDUCTOR NANOSTRUCTURES

Workshop brief summary in the following three areas:

1. Growth and nanomechanics;
2. Nanodevices and simulation;
3. Nanophysics and quantum phenomena.

In each of these areas, we highlight (a) open problems, (b) experimental achievements, (c) current-state-of-the-art modeling, and (d) feasibility of mathematical and computational methodologies.

I. Growth/Nanomechanics

1. Open Problems

    a. Reliable surface structure prediction beyond periodicity and reliable prediction of predictions
    b. Reliable growth process control and simulation (3D nucleation, defect control)
    c. Uniformity and quantity of a few nm materials

2. Experimental achievements
    a. Emerging nanoscale expt (3D atom precision probe method for positions and compositions, mechanical, thermal, optical, …)

3. Current state-of-the-art modeling
    a. Techniques: kMC, accelerated MD, longer time scale simulations, multiscale, multiphysics models, atomistic/continuum (DFT, level set, …)
    b. Current techniques cannot be used to design nanoscale structures and their properties

4. Feasibility of mathematical and computation methodologies
    a. Currently possible to simulate ~1000 atoms for DFT. Need ~1000000 for QD and Qwi.
    b. kMC for cluster distribution
    c. MD for diffusion
    d. continuum approach for surface morphology
    e. DFT for sticking coefficients

II. Nanodevices and Simulation

5. Open Problems
    a. Control of carrier injection, and photons and phonons
    b. Realistic and reliable device modeling
    c. Coherence/decoherence

6. Experimental achievements
    a. Multicell junction and core-shell solar cells
    b. Entangled photon states
    c. DNA sensitive FETs

7. Current state-of-the-art modeling
    a. 50+ million atoms + VFF
    b. Time-dependent DFT
    c. quantum MC

8. Feasibility of mathematical and computation methodologies
    a. Multiphysics modeling of nanostructures
    b. Multiscale techniques from atomistic level to the device level
    c. NEGF techniques for transport

III. Nanophysics and Quantum Phenomena

9. Open Problems
    a. Reduction for decoherence
    b. Quantum system identification
    c. Measurement in quantum physics
    d. Strongly correlated quantum systems
    e. Quantum transport phenomena in complex systems

10. Experimental achievements
    a. Single photon emission
    b. Single-electron spin detection
    c. Demonstration of coherence
    d. Quantum spin Hall effect

11. Current state-of-the-art modeling
    a. DFT relaxation + TB electronic structure
    b. Ab initio and temporal behaviour
    c. NEGF

12. Feasibility of mathematical and computation methodologies

Outcome of Workshop

- ❖ Networks created across disciplinary borders
- ❖ Recognition of physics and mathematics driven nanoscale modeling
- ❖ Consensus-building towards real-time simulation for design and control of nanostructures and devices