# Kyeongjae Cho

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### Professional Preparation

Ph.D. - Physics Massachusetts Institute of Technology - 1994

M.S. - Physics Seoul National University, Korea - 1988

B.S. - Physics Seoul National University, Korea – 1986

# Research Areas

#### Nanomaterials for renewable energy application

Limited supply of fossil fuels and environmental pollution issues require renewable energy technology using hydrogen as energy carriers. Three key technology components are hydrogen production, storage, and utilization in fuel cells. At the core of the renewable energy technology research is new materials to convert energy from one form to another (e.g., photon energy to electricity in solar cell, or chemical energy to electricity in fuel cell). There are extensive research efforts to develop new nanomaterials with higher efficiency in the energy conversion and optimized functional properties, but most of them are driven by empirical trial-and-error material development process. Computational modeling can provide detailed understanding on the microscopic mechanisms and properties nanomaterials for diverse applications. Our research is to apply molecular dynamics and Monte Carlo simulations to identify atomic structures of nanoscale materials and use quantum simulations to investigate functional properties through electronic structure analysis. Target materials systems are carbon nanotubes, semiconductor nanowires, metal nanoparticles, and oxide nanomaterials in diverse functional nanocomposite nanomaterials.

### High-k gate stack technology

Device scaling is leading to sub 32nm device feature size and continuous scaling requires new device materials such as high-k gate dielectric (replacing silica), metal gate electrode (replacing doped poly-silicon), and high mobility channel materials (e.g., Ge or compound semiconductors replacing silicon). These new device materials form interfaces and the interface properties critically control the device performance. These interfaces are very thin (nm scale), and computational modeling can provide critical insight to solve many technological challenges in developing the high-k gate stack as future device technology. Our research will apply atomistic modeling method to determine the atomic

structure of the interfaces and quantum mechanical simulations to calculate the electronic structures. The analysis of simulation results would provide detailed insights on the nano-scale structure-property relationship of high-k gate stack materials.

# Research Interests

Computational modeling study of nanomaterials with applications to nanoelectronic devices and renewable energy technology.