

## Seminar

# Predictive modeling of low-dimensional materials, synthesis to properties

**Boris I. Yakobson**

*Department of Materials Science & NanoEngineering,  
Department of Chemistry, and the Richard E. Smalley Institute,  
Rice University, Houston, USA*

### Abstract

Comprehensive tools of materials modeling allows one to make verifiable predictions of novel physical structures with specific, often useful or even extraordinary, properties. Recent examples from our work at my Rice University (Fig. 1) lab will be presented. First, an outline of evolutionary selection growth of monocrystal achieved for