Reasons for computational modeling
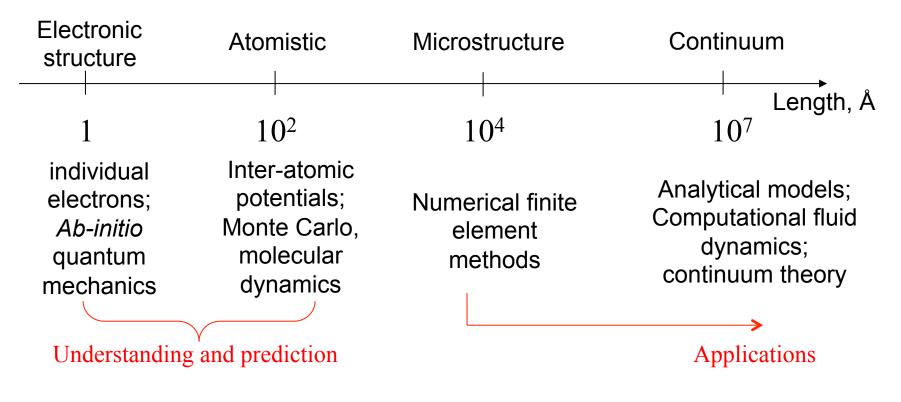
1. To interpret experimental data

2. To gain a deeper, microscopic understanding of materials and their macroscopic behavior via controlled modeling

3. To predict physical/chemical properties of materials prior to experiments (**inverse band structure approach**)

Length Scales in Materials Modeling

Electronic structure	Atomistic	Microstructure	Continuum
1	10^2	10^4	10^7
individual electrons; *Ab-initio* quantum mechanics	Inter-atomic potentials; Monte Carlo, molecular dynamics	Numerical finite element methods	Analytical models; Computational fluid dynamics; continuum theory

Length, Å

Understanding and prediction

Applications