Joint Institute for Nanoscience

The Quasi-continuum Theory for Nano Structures

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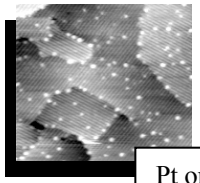
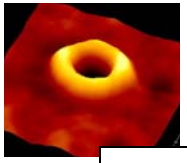
The quasi-continuum theory is a seamless multiscale modeling approach offering atomic scale resolution in high energy regions, and reduced atomic representation otherwise. The approach enables the treatment of material volumes approaching a billion atoms, and captures the effects of nanoscale strains on the structure and properties.

Challenges for Modeling Nanostructures



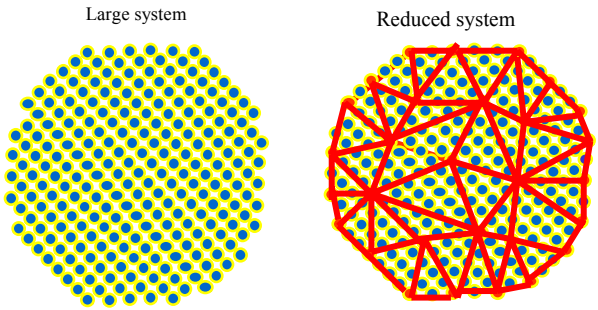
Pt on TiO_2



Cu_2O rings on $SrTiO_3$

- Large numbers of atoms, up to ~billions
- Need to deal with host phase
- Strong heterogeneity (atomic and phase scales)
- Need new classes of interatomic potentials
- Need novel methods for treating long range interactions (self-organization)
- Certain properties must be determined with electronic scale resolution
- Nanoscale strain impacts structure and properties

Idea of Quasi-continuum Theory



$$\min_{q} \Phi(q) \Longrightarrow \min_{q_R} \Phi(q_R) \quad \text{where} \quad q_R \subset q$$

- Reduction of the system is achieved by introducing kinematic constraints on the atomic displacements
- Coarse-graining of the fully atomistic method, with interatomic potential representing the fundamental input