Molecular Modeling of Nanocomposites
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1D- Clay Minerals
- Clay Minerals are hydrous aluminum phyllosilicates.
- Have variable amount of iron magnesium alkali metals and other cations.
- Typical MMT have net charges distributed within the octahedral layer or tetrahedral layer.
- Bulk Modulus: ~ 20-50 GPa
- Young’s Modulus: ~ 6.2 GPa

2D- Carbon Nanotube
- Single-walled Carbon Nanotubes & Multwall Carbon Nanotubes
  - Diameter: ~ 1 nm
  - Length: ~ 100 μm
- Superior Mechanical Properties
  - Elastic Modulus: ~ 1 TPa
  - Density: ~ 1/6th of steel
  - Conductive Ability: ~ 100,000 times that of copper
- Yield Strain: More than 4%
- Buckling Strain: ~ 5% (aspect ratio of 1/6)

2D- Graphite & Graphene
- Single carbon layer and multi carbon layers
- Thickness: ~ 5-10 nm
- Length: ~ 0.86-15 μm
- Superior Mechanical Properties
  - Elastic Modulus: ~ 1 TPa
  - Intrinsic Strength: ~ 130 GPa
  - Young’s Modulus: ~ 200 GPa

3D- POSS Organic-Inorganic Nanocomposites
- A new class of organic – inorganic nanocomposites containing POSS monomers which have been copolymerized with organic monomers.
- POSS hybrid chemical composition
- Superior Mechanical Properties
- POSS molecules span 1-3 nm size range
- Improve impact resistance.
- Reduce friction and improve flow.
- POSS can dissolve in polymers.

Molecular Dynamic Simulation of Nanocomposites and their Constituents

Parametric Evaluation of Multiwalled Carbon Nanotubes (MWCNT) MD

I. Geometrical Parameters
  A. Chirality
  B. Number of Carbon Nanotube Walls
  C. Aspect Ratio

II. Simulation Parameters
  a) Temperature Effect
  b) Thermodynamic Ensemble
  c) Thermostat and Barostat Algorithm

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