

## Data origin

- experiments
- informatics (data science)
- simulations
- theory

## Materials types

- organic compounds
  - o alkanes
  - o alkenes
  - o alkynes
  - o alcohols
  - o aldehydes
  - o amines
  - o carboxylic acids
  - o cycloalkanes
  - o cyclic compounds
  - o esters
  - o ketones
  - o nitriles
- polymers
  - o copolymers
  - o elastomers/rubbers
  - o homopolymers
  - o liquid crystals
  - o polymer blends
  - o thermoplastics
  - o thermosets

Note: All of the above entries can be further described further:

- (reference to standard notation, IUPAC, or link to PubChem)
- Trade name (if a commercial material)
- Polymer class (use one of following based on the chemical structure of constitutional unit (CU) of polymer)
  - Polyacrylics
  - Polyamides / thioamides
  - Polyhydrides / thiohydrides
  - Polycarbonates / thiocarbonates
  - Polydienes
  - Polyesters / thioesters
  - Polyhalo-olefins
  - Polyimides / thioimides
  - Polyimines
  - Polyketones / thioketones

- Polyolefins
  - Polyoxides / ethers/acetals
  - Polyphenylenes
  - Polyphosphazenes
  - Polysiloxanes / silanes
  - Polystyrenes
  - Polysulfides
  - Polysulfones / sulfoxides / sulfonates / sulfoamides
  - Polyurethanes / thiourethanes
  - Polyureas / thioureas
  - Polyvinyls
- Molecular weight
- Processing compositions (hardener, additive)
- Polydispersity
- polymer composites
  - fiber-reinforced
  - nanocomposites
  - particle-reinforced
  - polymer-matrix

Note: All of the above entries can be further described further:

- Particle type (E.g., spheroidal, platelet, fiber)
- Particle Composition (E.g., chemical composition of particle)
- Particle surface functional groups (E.g., siloxanes, -OH groups)

### **Structural features**

- defects
  - bubble of gas
  - crazing
  - debonding
  - disclinations
  - dislocations
  - particle agglomerates
  - pores
- interfacial
  - interfacial surface area
  - interfacial tension/energies
  - interfacial thickness
- microstructures
  - body centered cubic spheres
  - defect structures
  - face centered cubic spheres
  - fractal dimension
  - gyroid

- hexagonally packed cylinders
- lamellae
- microemulsion
- particle dispersion/distributions, e.g. clustering
- particle shape
- perforated lamellae
- porosity
- molecular structure
  - alternating copolymer
  - block copolymer
  - bottlebrush
  - dendrimer
  - end-group composition
  - functionalization
  - gradient copolymer
  - linear
  - long-chain branching
  - number average molecular weight
  - polydispersity
  - polymer network
  - random copolymer
    - short-chain branching
    - star
    - statistical copolymer
    - statistical segment length (Kuhn length)
    - supramolecular
    - surfactants
    - tacticity
    - weight average molecular weight
- morphologies
  - aligned
  - amorphous
  - anisotropic
  - clusters
  - crystalline
  - dispersion
  - glassy
  - isotropic
  - percolated
  - porous
  - random
  - rubbery

- semicrystalline
- woven

### **Properties addressed**

- chemical
  - composition
  - functional ligand/surfactants
- durability
  - aging (Note: also used under **Synthesis and processing--Annealing and homogenization**)
  - water absorption (Note: also used under **Properties Addressed--Transport**)
- electrical
  - conductivity
  - current and energy density
  - dielectric breakdown strength
  - dielectric constant and spectra
  - dielectric dispersion
  - endurance strength
  - surface resistivity
  - volume resistivity
- magnetic
  - susceptibility
- mechanical
  - bulk (compressional) modulus
  - creep
  - deformation mechanisms
  - ductility
  - fatigue
  - flexural response, modulus
  - fracture behavior
  - fracture toughness
  - impact response
  - plasticity
  - Poisson's ratio
  - sheer modulus
  - strength
  - stress-strain
  - tensile response, modulus (Young's)
  - tensile strength
  - yield strength
  - viscoelasticity
- rheological

- intrinsic viscosity
- monomer friction coefficient
- viscosity
- thermodynamic
  - calorimetry profile
  - critical temperatures
  - crystallization temperature
  - degradation temperature
  - glass transition temperature
  - heat capacity
  - heat of fusion
  - interfacial energies
  - surface energies
  - melting temperature
  - specific heat
  - thermal conductivity
  - thermal decomposition
  - temperature
  - thermal expansion
- transport
  - density
  - gas permeation
  - water absorption

### **Characterization methods**

- mechanical
  - compression tests
  - creep tests
  - hardness
  - fatigue
  - in situ testing
  - measures of toughness
  - nanoindentation
  - shear or torsion tests
  - tension tests
- microscopy
  - atomic force microscopy
  - confocal microscopy
  - optical microscopy
  - scanning electron microscopy
  - scanning tunneling microscopy
  - transmission electron microscopy
- scattering and diffraction

- light scattering
- neutron scattering
- small angle X-ray scattering
- X-ray diffraction
- spectroscopy
  - dielectric
  - density mechanical analysis
  - Fourier-transformed infrared spectroscopy
  - nuclear magnetic resonance (NMR)
  - neutron spin echo spectroscopy
  - raman
- thermochemical
  - calorimetry
  - differential scanning calorimetry
  - differential thermal analysis
  - thermogravimetry

### **Computational methods**

- density functional theory
- discrete element method (DEM)
- discrete field approach
- dissipative particle dynamics (DPD)
- finite element analysis
- finite volume method (FVM)
- molecular dynamics (MD)
- Monte Carlo methods (MC)
- multiscale simulations
- phase field
- self-consistent field theory (SCFT)

### **Synthesis and Processing**

- Annealing and homogenization
  - aging
  - mechanical mixing
  - melt mixing
  - ultrasonication
- deposition and coating
  - electron beam evaporation (EBE)
  - physical vapor deposition (PVD)
  - solvent casting
  - spin coating
- forming
  - compression molding

- die casting
  - hot pressing
  - injection molding
  - milling
  - rotational molding
  - vacuum molding
- Mixing
  - dry blending
  - extrusion
  - twin screw extrusion
- powder processing
  - ball milling
  - hot pressing
- reactive
  - curing
  - dissolving
  - drying
  - in-situ polymerization
  - solution processing
- self-assembly
  - directed self-assembly
  - evaporation induced assembly
  - field directed self-assembly
  - micelles
  - monolayer
  - self-assembly-assisted grafting
  - surface directed self-assembly