Data Science on Materials

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Materials Database /

- A novel database containing an extensive array of compounds, materials and their properties has been created with help of students working in Florida International University.
Project statistics

- Total solid compounds: 3485
  - Elements (97)
  - Compounds:
    - Oxides (919)
    - Carbides (121)
    - Hydrides (739)
    - Nitrides (78)
Extent of Data

- As of three moths ago the element database contained data on 56 different elemental properties. The database covers all of the common general properties thermodynamic, structural, electronic and mechanical properties.

  - Element electronic properties
  - General properties
  - Magnetic properties
  - Mechanical properties
  - Optical properties
  - Structure properties
  - Thermal properties
### Extent of Data

#### Element electronic properties
- DHf negative ion
- EA Energy
- Electron Affinity
- Electronegativity
- Ionization Potential

#### General properties
- Weight
- Density
- Melting Point
- Boiling Point
- Physical form
- Critical point temperature
- Tripple-point temperature
- Solubility

#### Magnetic, electrical properties
- Magnetic Susceptability
- Resistivity

#### Optical properties
- Index of Refraction

#### Mechanical properties
- Bulk Modulus
- Compressibility
- Hardness, microhardness
- Brinell Hardness
- Vicker Hardness
- Rigidity Modulus
- Young Modulus
- Poisson Ratio
- Elastic Constants

#### Structure properties
- Structure
- Space group
- Pearson symbol
- Lattice parameters

#### Thermal properties
- ΔH Atomization
- Δ H Fusion
- Δ H Vaporization
- Δ S Fusion
- Δ S Vaporization
- Debye temperature
- Gibbs Energy
- Enthalpy
- Specific Heat, Molar Heat
- Heat of Sublimation
- Thermal Conductivity
- Thermal Expansion
- Lattice Energies
- Vapor Pressure
Sources of Data

Compound and element properties data was collected from reliable sources who can provide the original scholarly references.

Main sources of data:
CRC: General compound properties
FACT: thermodynamic data of compounds
ICSD: structure and crystal data of compounds
Demonstration

- A fast data mining application which could be used with our database has been written.

- Allows easy filtering and selection of required compounds and their properties.
- Search by type of compound, e.g. Oxide, Hydride, carbide
- Search by group or period, of composing elements
- Filter by phase, and or structure type
Future goals

The latest work which was not shown.

Work is in progress:
- Move to a more efficient relational database design.
- Provide public access to the database via internet.