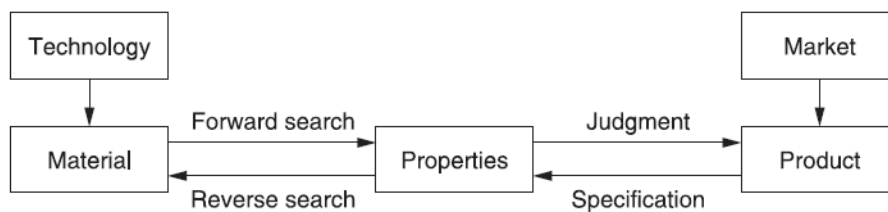


## HUBUNGAN ANTARA STRUKTUR DAN PROPERTY: METODE PENCARIAN DAN TANTANGAN

### Proses Membawa Produk Ke Pasar



Hubungan antara material dengan properties

## Tiga Parameter Penting dalam Desain Sebuah Produk

- Parameter Struktur
- Parameter Properti
- Parameter Pasar dan Lingkungan

## Parameter Struktur

### 1. Untuk komponen tunggal:

- a. parameter struktur meliputi proporsi atom dan konektivitas nya
- b. parameter geometri dan energi dari ikatan, sudut dan konformasi;
- c. Parameter elektronik meliputi distribusi elektron dan polarisasinya

### 2. Untuk Sistem Multi Komponen yang meliputi larutan, mikrostruktural material dan material komposit:

- a. Proporsi antar komponen
- b. Hubungan antar fase, misal koloid, larutan dan komposit

## Parameter Properti

- **Properti Fisik:** Keadaan materi, kesetimbangan fase, thermal, optical, mechanical, elektromagnetik
- **Properti Kimia:** Pembuatan, Reaktivitas, Reaktan dan produk, kinetika, Flash Point dan explosion limit
- **Properti biologi:** Toksikitas, pengaruh fisiologi dan farmakologi, nilai nutrisi, bau dan rasa

## Parameter Pasar dan Lingkungan

- **Pasar:** Area pemakaian, volume penjualan, harga, potensi pertumbuhan
- **Lingkungan:** Transportasi dan Transformasi, konsentrasi, keselamatan, kesehatan dan dampak lingkungan

## Forward Search from Material to Property

1. Find the structure parameters  $x$  and the properties  $y$  of a given compound at room temperature and pressure. What are the properties of the compound at elevated or lowered temperatures and pressures, as well as of other environmental variables, such as electromagnetic field and solar radiation, so that this search can be written as  $y = f(x, T, P)$ ?
2. When the lead compound is subjected to various chemical and physical modifications, what are the various families of derivative materials that can be made with this technology, where the derived structure can be written as  $x + \Delta x$ ?
3. What are the properties of these derivative materials,  $y + \Delta y$ ? The derivative  $\Delta y/\Delta x$  is of particular interest, as it represents the property modifications resulting from structure modifications. This knowledge would be useful in exploring ways to improve product properties.

## Search Methodologies

### 1. Literature Search

- Textbook
  - Handbook
  - Research Journal ←
  - Electronic Resource
- First publication of  
property related  
materials

Chemical compound name → its molecular structure  
→ Its physical and chemical properties

## Prediction From Theory

Material → Property

Can it be predicted from theory?

Need computational:

- Ab initio method (start from Schrodinger equation)
- Semi-empirical method (ignore core electrons and consider only the outer shell)
- Molecular Mechanics (Modeling of molecule as a number of atoms connected together by flexible bonds)

## Prediction by Correlation

**Quantitative correlation** can be predicted by **large and systematic data base** → **need theoretical justification**

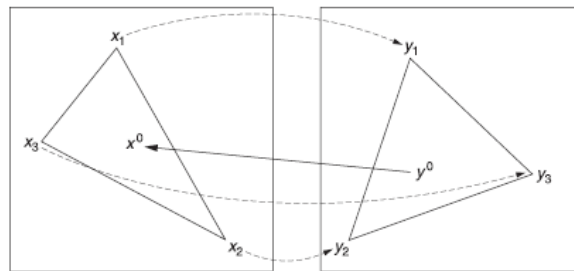
→ Simple method → Linier function or multilinier combination

→ More reliable to intrapolate than extrapolate

→ **Group contribution method** → predict property based on the groups

## Reverse Search from Property to Material

- Literature
- Forward search plus interpolation



- Random Search

## Search from Technology to Markets

We have powerful technology to make material with interesting properties

→ Find market

## Literature and Database

- Books, Handbooks and References
- Journal and catalogs
- Electronic database
- Spreadsheets and database
- CD-ROMs and Floppy Disks
- Internet Databases

## Exercises

1. Do a forward search from materials to properties. Find the boiling points and melting points of 1-alcohols from  $C_1$  to  $C_{20}$ .
  - (a) Make a table for these properties.
  - (b) Make a plot of these properties versus the number of carbons  $N_C$ .
  - (c) Compare this plot with the normal paraffins.
2. Make a table of the densities, boiling points, and melting points of the first 54 elements.