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150 years



We create chemistry

Computational Science in the Chemical Industry

Roel Sanchez

Staff Chemist, Quantum Chemistry

PUBLIC

Agenda

- **Introduction**
- Research at BASF
- Modeling at BASF
- Trends & Collaborations

Innovation

Research and development at a glance

Research for the future: with our innovative products and processes, we provide sustainable solutions for global challenges.

- Expenditures for research and development €1,884 million, world leader in chemical industry
- Around 3,000 projects
- Strongest innovation power in the chemical industry (No.1 in the Patent Asset Index™)
- Targets 2020:
around €30 billion sales and around €7 billion EBITDA from innovations



1	Chemicals	10 %
2	Performance Products	19 %
3	Functional Materials & Solutions	20 %
4	Agricultural Solutions	27 %
5	Oil & Gas	3 %
6	Corporate Research, Other	21 %

Innovation Global Know-How Verbund

150 years

 **BASF**
We create chemistry

Thanks to our close cooperation with numerous partners in science and industries worldwide, we have created an international and interdisciplinary Know-How Verbund.

- Approx. 10,700 employees in research and development worldwide
- Know-How Verbund with around 600 excellent universities, research institutions and companies



150 years

 **BASF**
We create chemistry

Demographic challenges set the stage for the future of the chemical industry

In 2050: More than nine billion people **but** only one earth



Chemistry as enabler

150 years



Chemistry-based innovations

Growth and technology fields

Global needs

Resources,
Environment
and Climate

Food and
Nutrition

Quality of Life

Customer industries



Transportation



Agriculture



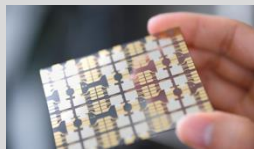
Construction



Energy & Resources



Consumer Goods



Electronics



Health & Nutrition

Growth fields

Automotive Lightweight
Composites

Batteries for Mobility

Enzymes

E-Power Management

Functional Crop Care

Heat Management
for Construction

Organic Electronics

Plant Biotechnology

Water Solutions

Wind Energy

...

Technology fields

Materials,
Systems &
Nanotechnology

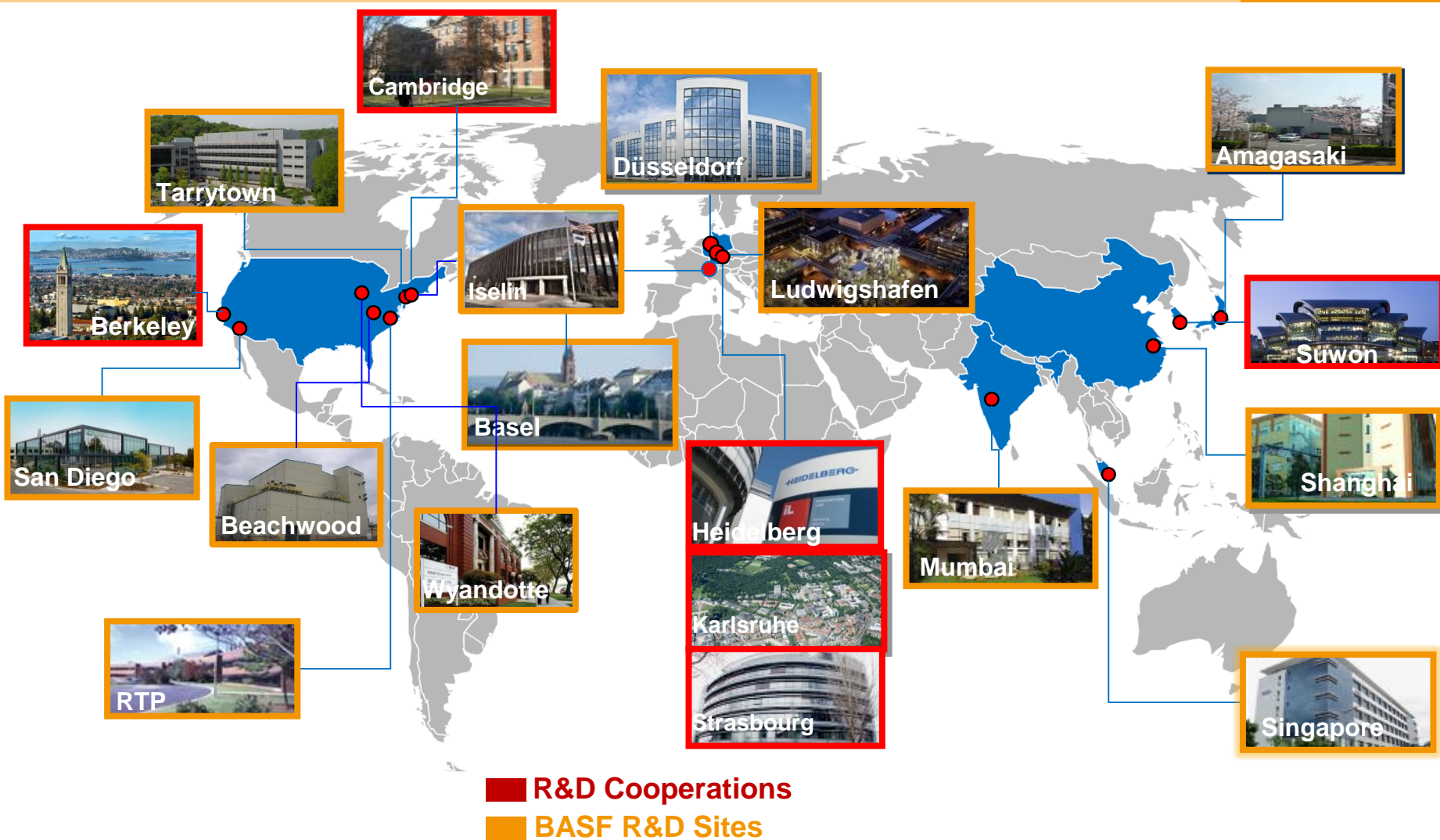
Raw Material
Change

White
Biotechnology

150 years

 **BASF**
We create chemistry

Global Organization – Regional Network



150 years



BASF in North America



Headquarters: Florham Park, NJ

2013 sales: \$19.3 billion

Employees: ~17,000

Prod. sites: ~100

Key customer industries:

- Agriculture
- Alternative Energy
- Automotive ● Chemicals ● Coatings
- Construction ● Health & Beauty
- Packaging ● Transportation

Agenda

- Introduction
- Research at BASF
- **Modeling at BASF**
- Trends & Collaborations

Modeling Research

Molecules, Materials, Systems, Processes

150 years



Teams:

Crop Protection
Modeling

Plant Science
Crop Trait
Knowledge

Emission
Catalysts Testing
and Modeling

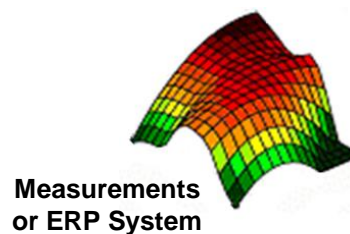
Computational
Fluid Dynamics

Materials
Modeling

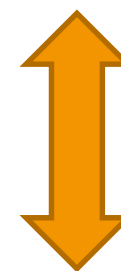
Mathematical
Optimization

Others...

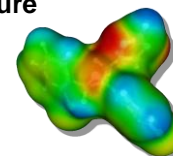
Approaches:



Empirical
Modeling

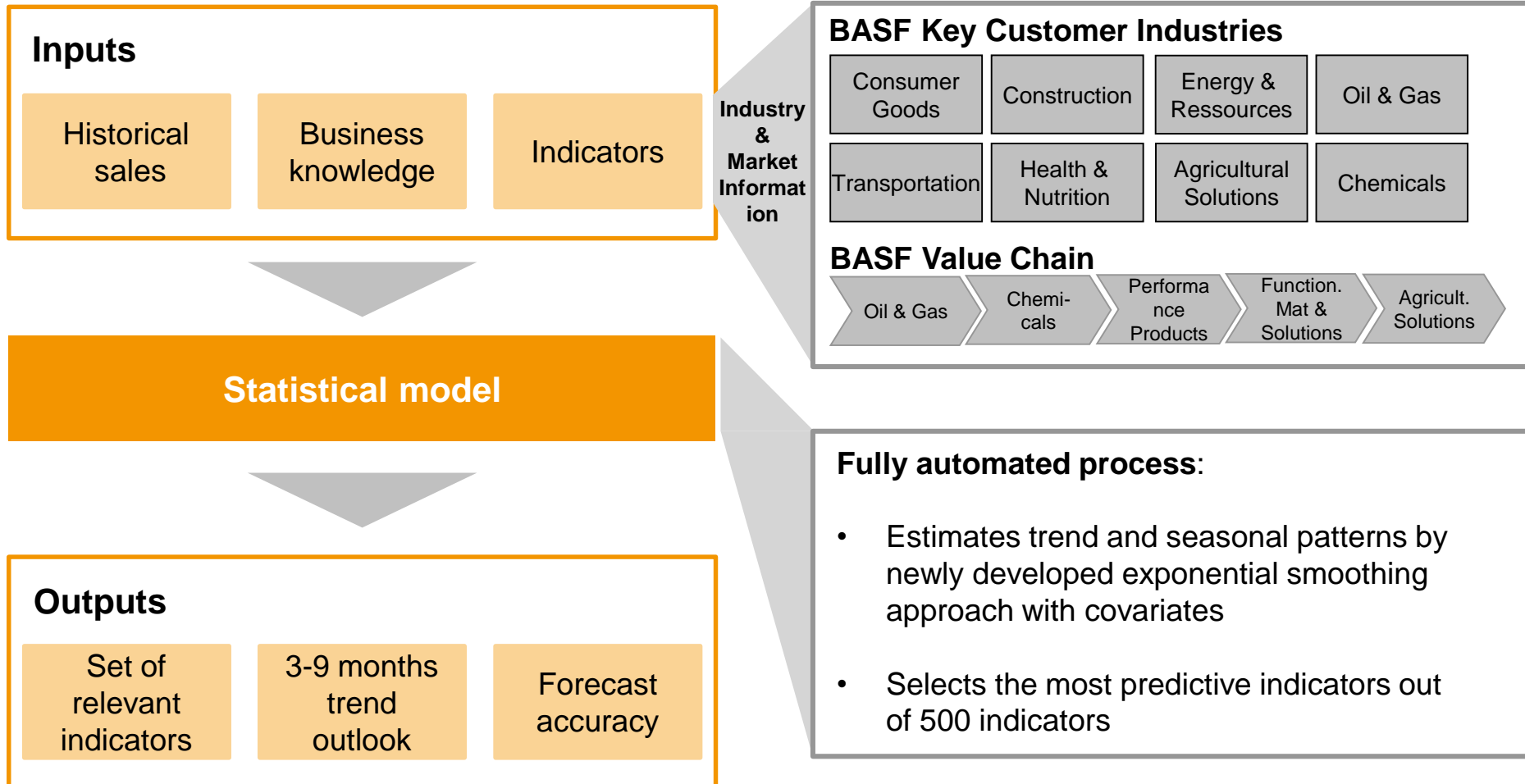


Laws of Nature



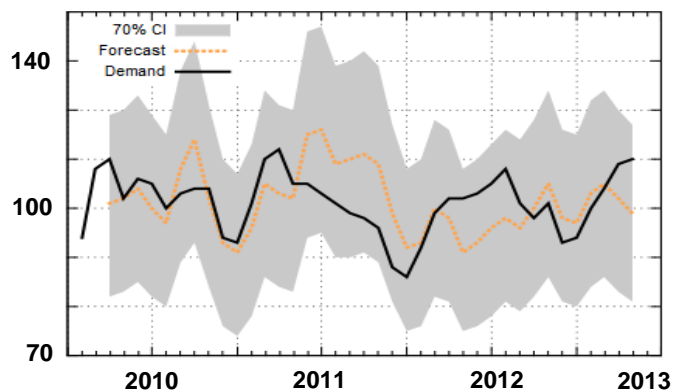
Fundamental
Modeling

Supply Chain Early Warning System Approach



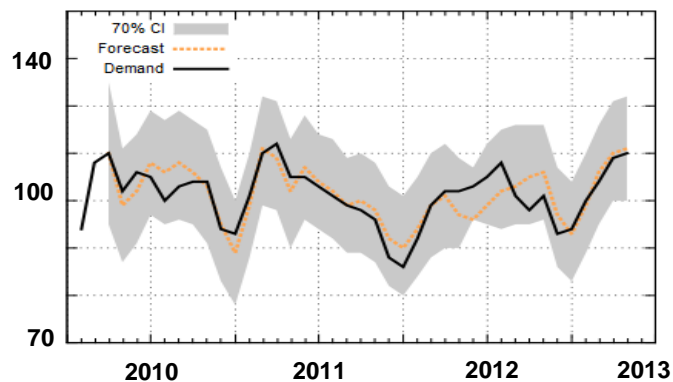
Supply Chain Early Warning System Result

Model based on history only

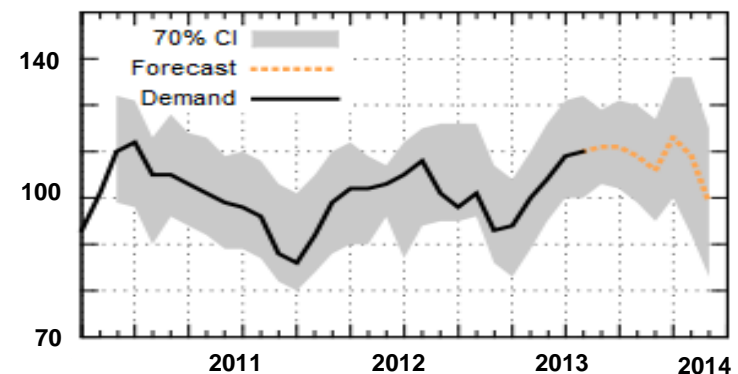


- Our approach outperforms statistical methods based on history only
- Forecast better captures the actual demand
- Forecast has lower prediction uncertainty
- Model allows prediction of potential impact of economic trends

Model with additional information



Forecast



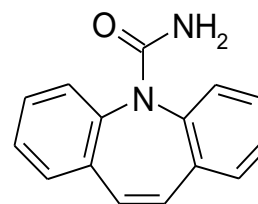
Quantum Chemistry ...

... is the calculation of **molecular** structures, properties and reactions with quantum mechanical methods (“*ab initio*”)

... uses computers (Linux clusters) as virtual laboratories

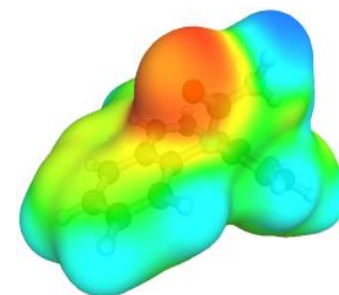
... helps in **understanding, quantifying, predicting**

- Intermolecular & surface interactions
- Electronic & physical properties
- 3D structure on atomic scale
- Chemical reactions
- Spectroscopy



Formula

QC

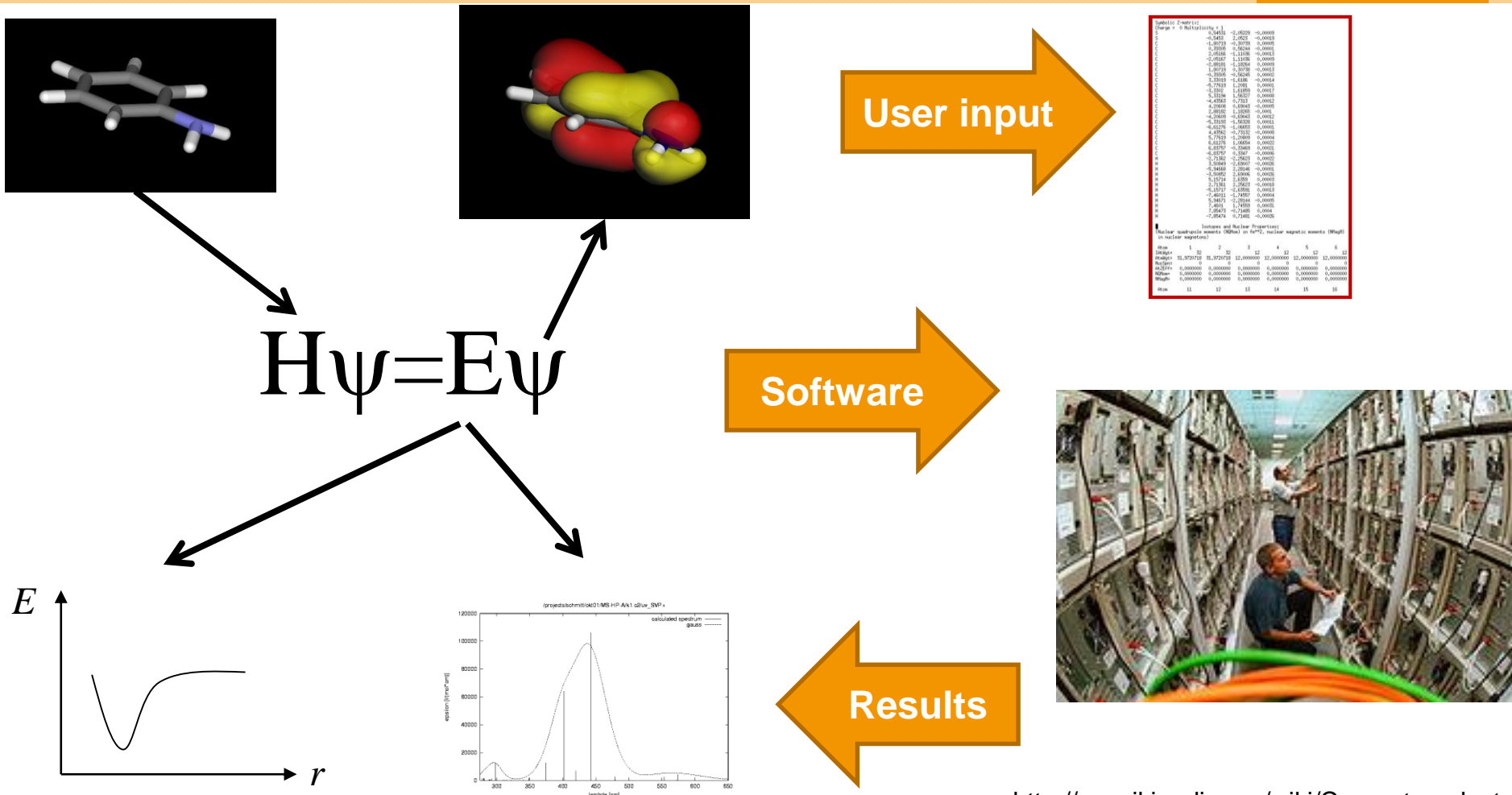


3D structure &
electron distribution

... generates ideas for **better products and processes**



Computational Quantum Chemistry: Solving the Schrödinger Equation



Agenda

- Introduction
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- **Trends & Collaborations**

Future Developments



New Application Areas Beyond
R&D, e.g. Marketing & Sales



Internal Partnering:
Early and Close Interaction



External Partnering:
Pilot Projects with Universities



basf.com/career



We create chemistry