150 years

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Computational Science in the Chemical Industry

Roel Sanchez

Staff Chemist, Quantum Chemistry

Agenda

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

Innovation
Research and development at a glance

150 years

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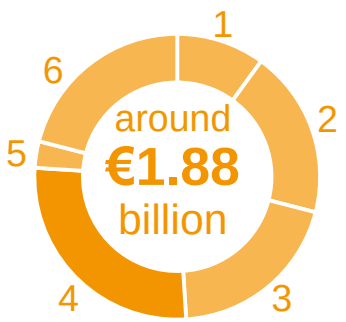
Research for the future: with our innovative products and processes, we provide sustainable solutions for global challenges.

- 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

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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

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

150 years

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

Chemistry as enabler

Chemistry-based innovations
Growth and technology fields

150 years

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Global needs

Resources, Environment and Climate

Food and Nutrition

Quality of Life

Customer industries

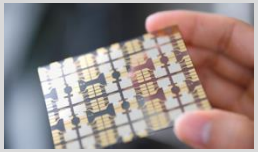

Transportation


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

Global Organization – Regional Network

150 years

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150 years

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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

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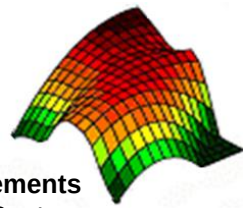
Teams:

- Crop Protection Modeling
- Plant Science Crop Trait Knowledge
- Emission Catalysts Testing and Modeling
- Computational Fluid Dynamics
- Materials Modeling
- Mathematical Optimization
- Others…

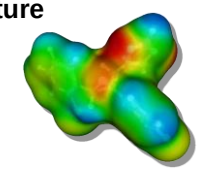
Approaches:



Measurements or ERP System

Empirical Modeling

Laws of Nature



Fundamental Modeling

Supply Chain Early Warning System
Approach

150 years

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Inputs

- Historical sales
- Business knowledge
- Indicators

Industry & Market Information

BASF Key Customer Industries

Consumer Goods	Construction	Energy & Ressources	Oil & Gas
Transportation	Health & Nutrition	Agricultural Solutions	Chemicals

BASF Value Chain

Oil & Gas → Chemi-cals → Performance Products → Function. Mat & Solutions → Agricult. Solutions

Statistical model

Fully automated process:

- Estimates trend and seasonal patterns by newly developed exponential smoothing approach with covariates
- Selects the most predictive indicators out of 500 indicators

Outputs

- Set of relevant indicators
- 3-9 months trend outlook
- Forecast accuracy

Supply Chain Early Warning System
Result

150 years

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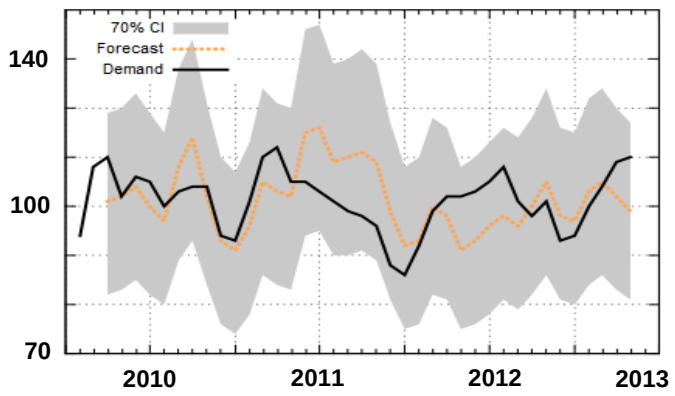
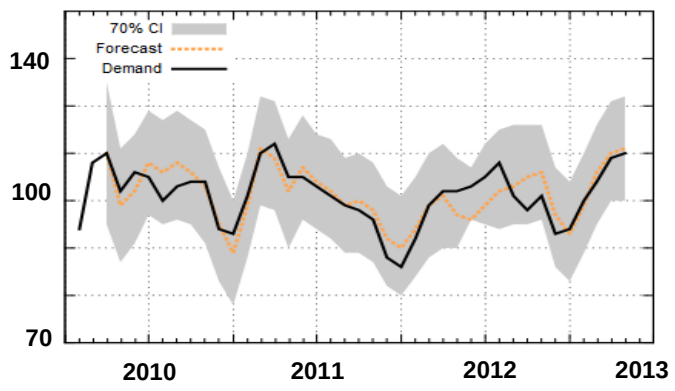
Model based on history only

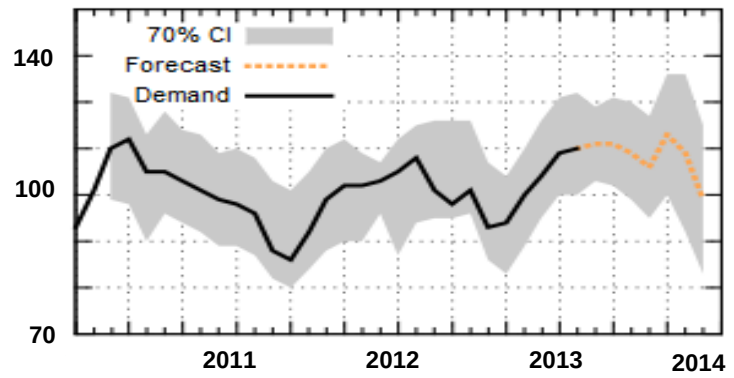


- Our approach outperforms statistical methods based on history only
- Forecast better captures the actual demand
- Forecast has lower prediction uncertainty
- Model allows prediction of potential impact of economic trends

Model with additional information



Forecast



Quantum Chemistry …

150 years

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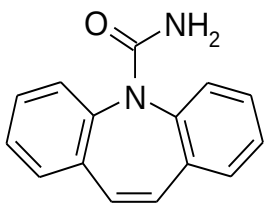
… is the calculation of **molecular** structures, properties and reactions with quantum mechanical methods ("*ab initio*")

… uses computers (Linux clusters) as virtual laboratories

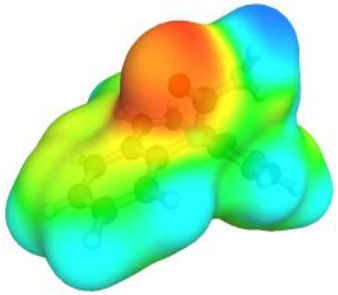
… helps in **understanding, quantifying, predicting**

- 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

150 years

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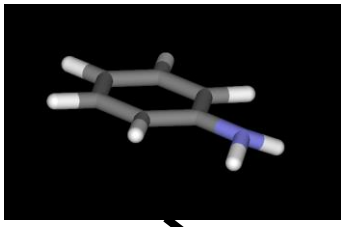
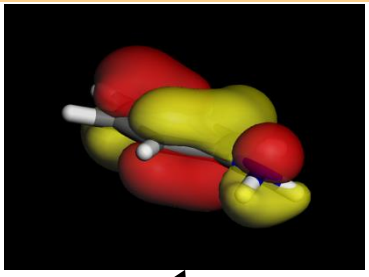
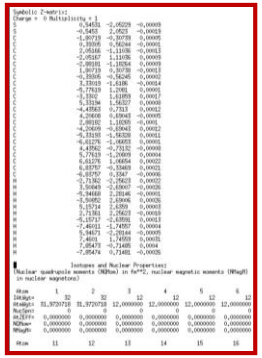


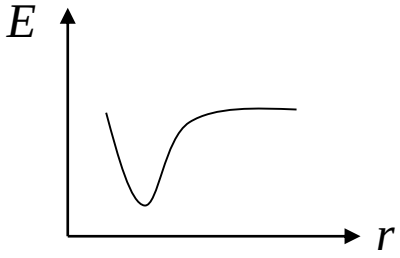


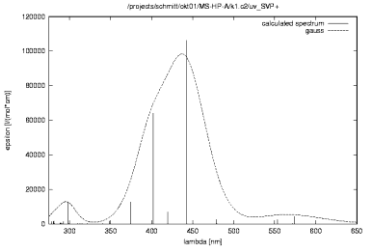
$$H\psi = E\psi$$

User input



Software





Results

http://en.wikipedia.org/wiki/Computer_cluster

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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

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