Reviewing the role of synchrotrons for Sasol

Relevance of research at synchrotrons for African Industries

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Sasol Group Technology

November 2015

sasol

reaching new frontiers

We are deeply shocked at the recent terrorist attacks in France. Our heartfelt condolences to all of those who have been affected.

Admire your courage to continue and host the conference.

We will use this opportunity to grow and expand our scientific networks.

Share our journey towards XRD & synchrotron

Ingredients:

1. Sustainable value creation
2. Leverage international footprint
3. Developing people
4. Enhancing stakeholder relationships
5. Technologies requiring research support
6. Challenging research questions
7. A solid home base
8. Prove synchrotron & neutron applications
9. Continuous implementation of synchrotron gained knowledge
10. Grow synchrotron knowledge
11. Advance Intellectual Property
12. Compose an analytical symphony

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Reviewing the role of synchrotrons in Sasol

- ***Ingredient 1: Sasol creates value***

Key inputs

	2015	2014	2013
Coal (kilotons)	**17 674**	17 555	17 896
Crude oil (mm bbl)	**33**	30	25
Natural gas (bscf)***	**134**	190	174
Water (thousand cubic metres)***	**135 458**	149 552	147 001
Total energy usage (thousand GJ)*/***	**413 838**	425 257	427 802
Oxygen (kilotons)***	**12 711**	14 907	15 017
Nitrogen (kilotons)***	**718**	1 356	3 527
Other (eg chemicals) (kilotons)***	**5 136**	6 358	6 892
Land area used (hectares)	**6 629****	5 245**	4 518

* Includes electricity usage, of which 70% is self generated.

** The increase in area affected by operations is due to the inclusion of two new mine projects: Impumelelo and Shondoni.

*** Decrease due to the sale of Solvents Germany and exclusion of the ORYX GTL data.

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Ingredient 2: Leverage international footprint.

- Sasol business has an international footprint.
- Experience in liaising with international companies.
- Develop & commercialise chemical technologies.
- Build & operate world-scale facilities.
- Produce range of high-value product streams:
  - Liquid fuels,
  - Chemicals.
  - Low carbon electricity.

The map reflects a broad indication of Sasol's global presence.

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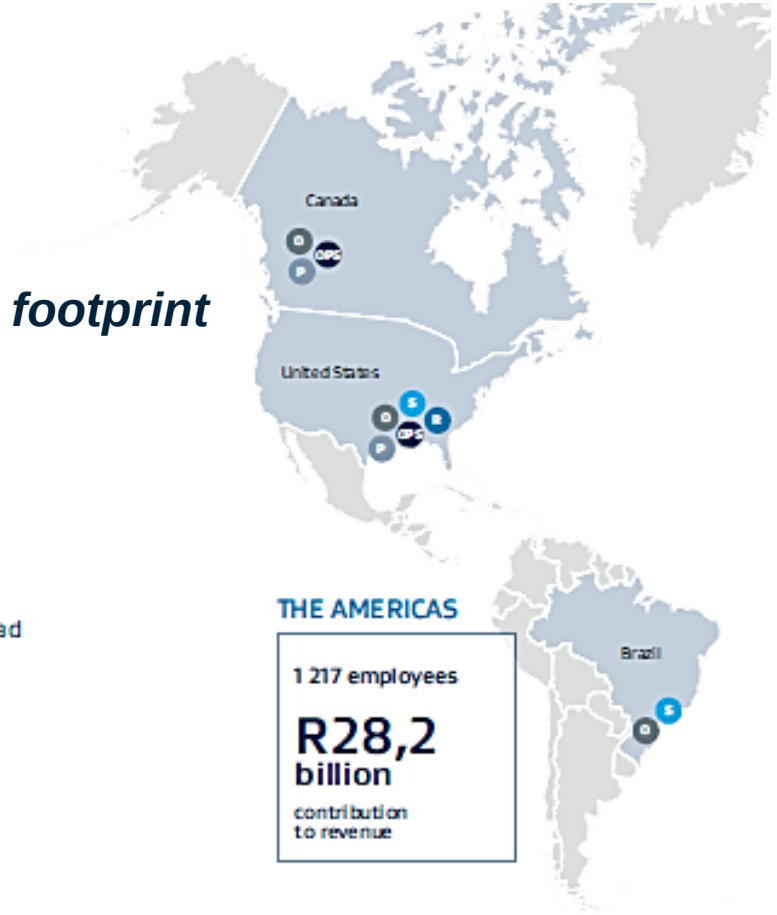
Ingredient 2:

Leveraging our international footprint



Our financial reporting reflects the broad regions in which we have a presence.

Profit from operations for 2015
R46,5 billion

Total capital investments for 2015
R45,1 billion
44% spent in South Africa

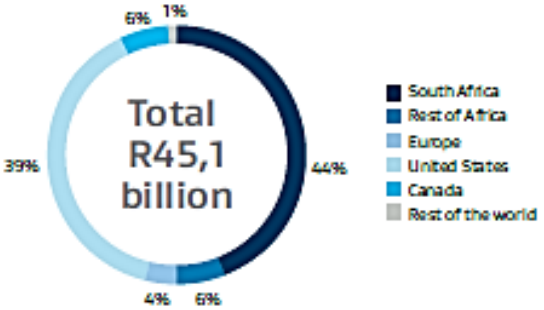
THE AMERICAS

1 217 employees

R28,2 billion

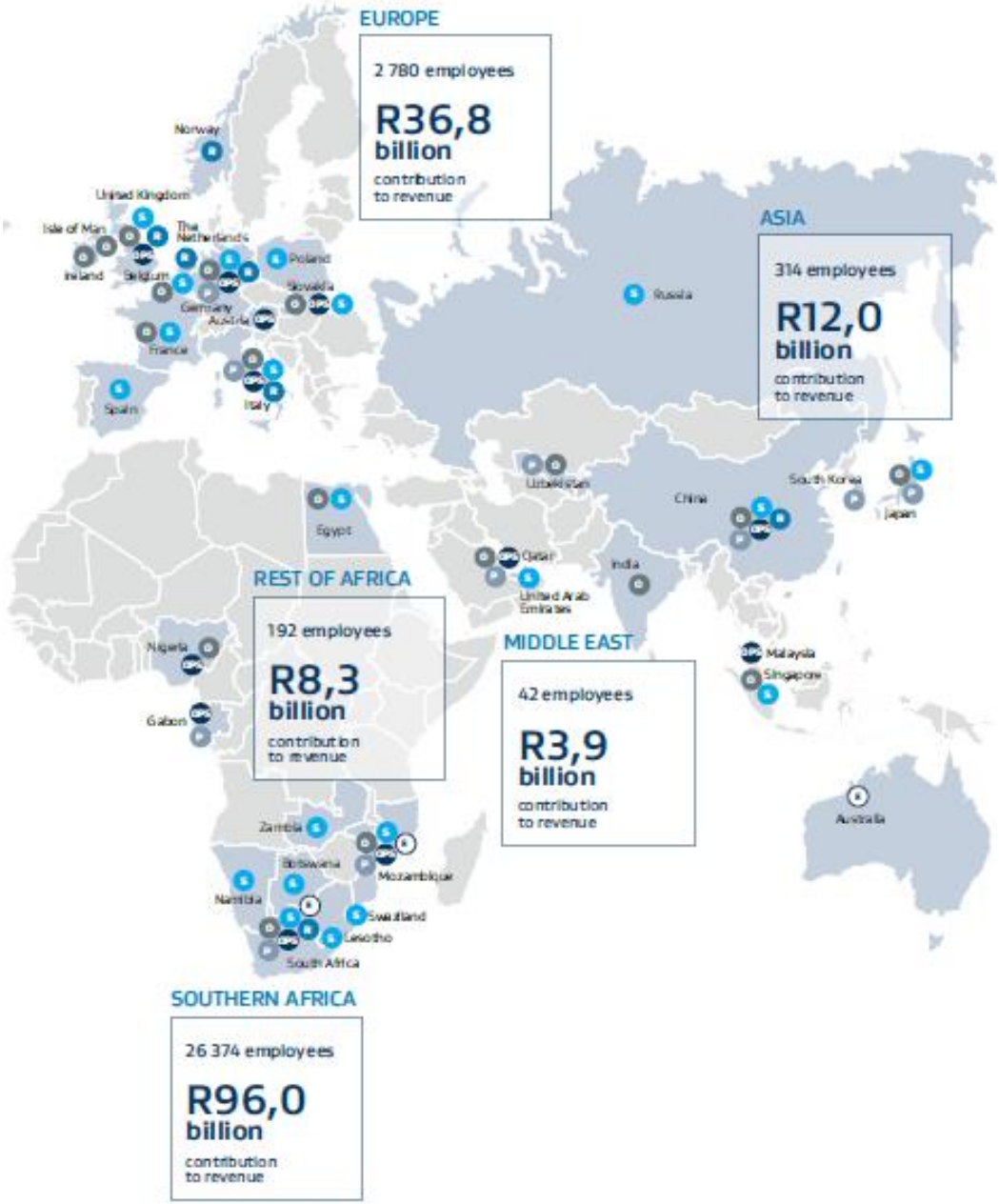
contribution to revenue

Capital investments by region for 2015



Legend

- Office
- Operations
- Sales
- Projects at the pre-feasibility, feasibility or implementation phase
- Research activities
- Exploration



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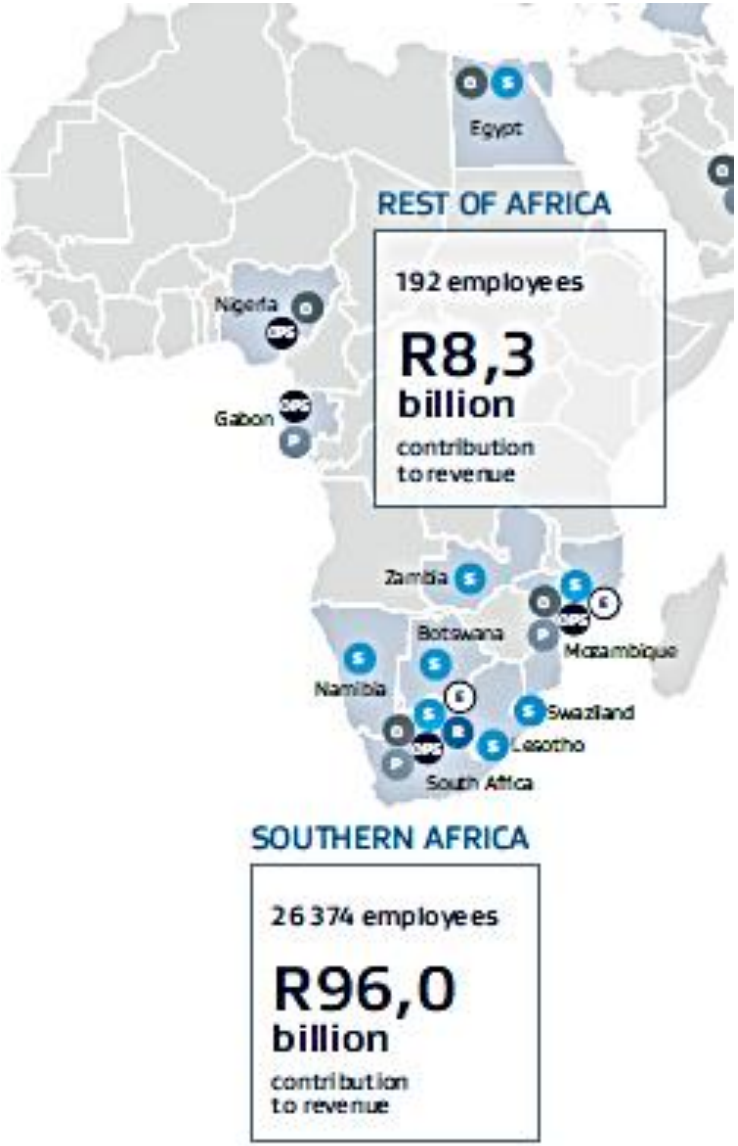
Ingredient 2:
Leveraging our international footprint

Near-to-medium-term strategy:
A largely dual-regional focus that seeks to leverage our global presence for **growth and expansion**.
Across our existing global footprint, we aim to **maintain and enhance** our asset base to make our plants more efficient and effective.

Ingredient 2: Leveraging our SA & African footprint



30 September 2015:

Capital spend of R19.8 billion

R 1.1 billion on skills and socio-economic development

R 34.7 billion in direct and indirect taxes

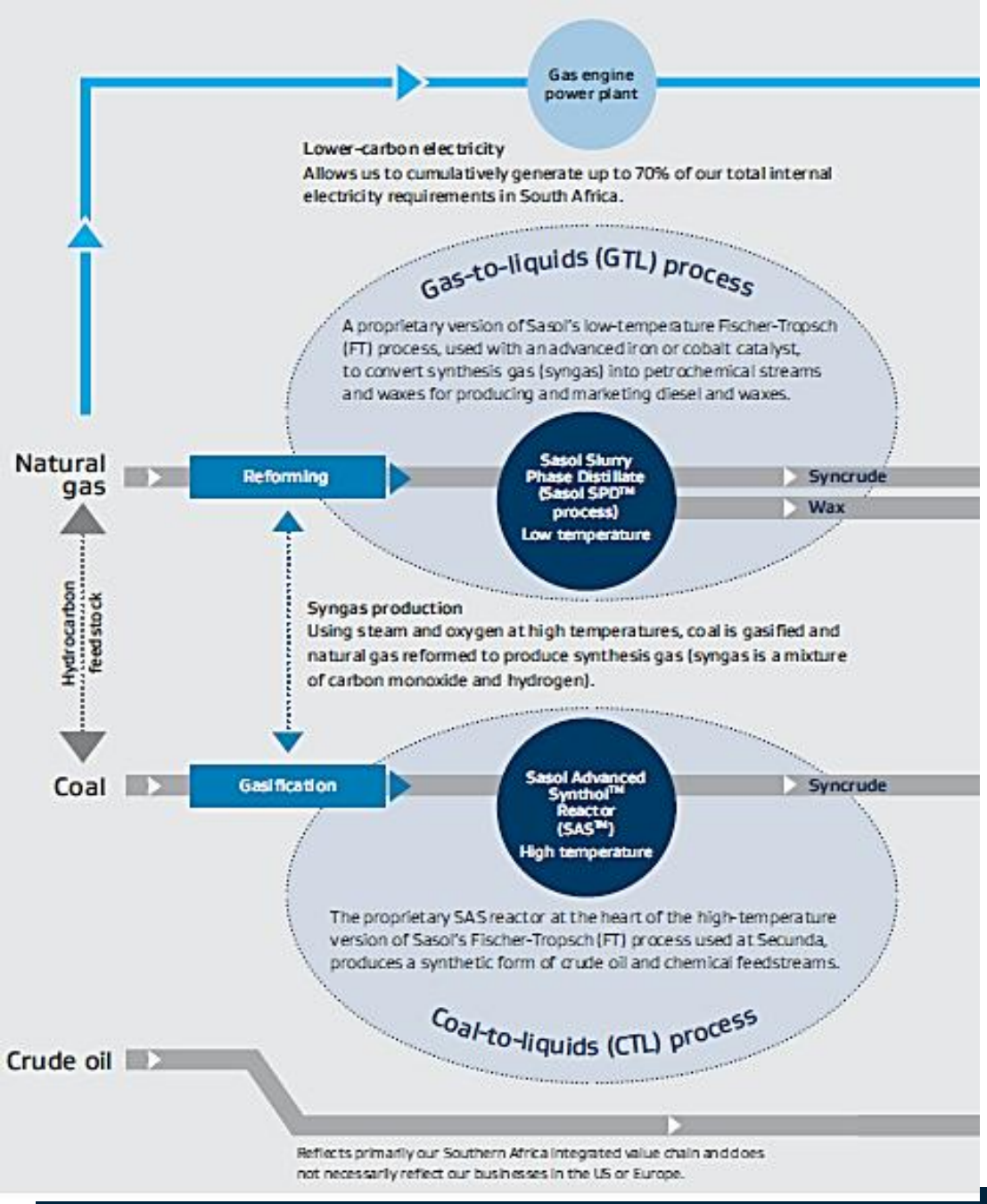
Ingredient 3: Developing people

Key outputs

	2015
Number of employment opportunities provided	30 919
Investment in employee learning	R692m
Number of employees receiving artisan training and external technical skills development	542
Number of employees receiving leadership training	2 872
Number of employees and contractors receiving HIV screening, counselling and testing	7 739

Ingredient 4: Enhancing stakeholder relationships

	2015	2014	2013
Economic value added	**R82,4bn**	R85,9bn	R73,9bn
Amount paid in government tax globally	**R10,1bn**	R12,9bn	R11,3bn
Investment in socioeconomic development and external skills development initiatives	**R1,2bn**	R1,4bn	R1,4bn
Broad-based black economic empowerment status*	**Level 4**	Level 3	Level 4



Ingredient 5: Technologies requiring research support.

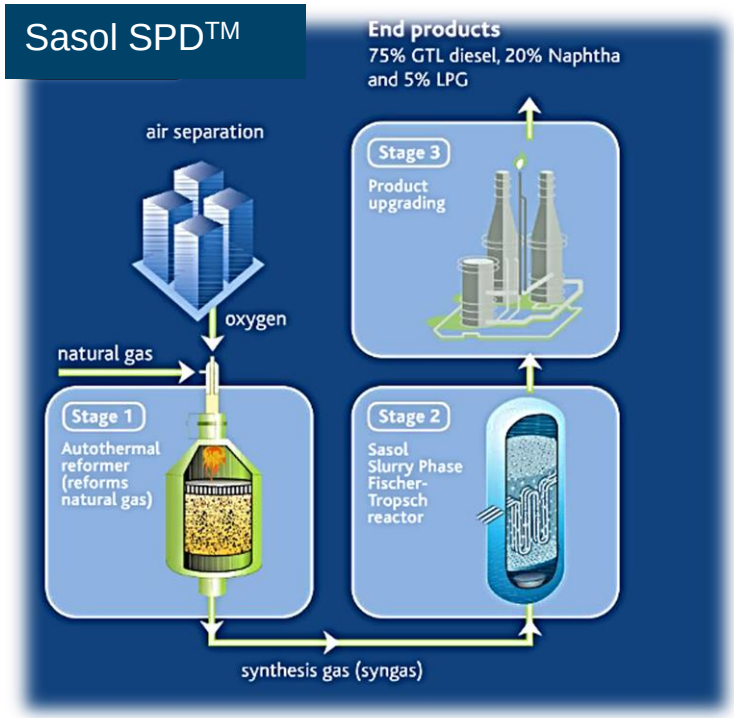
syncrude
wax

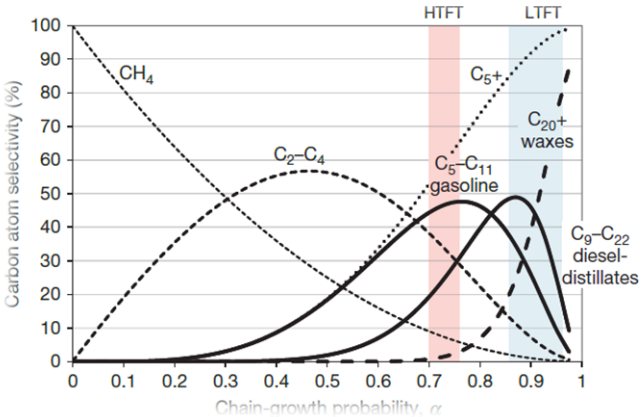
Ingredient 5: Technologies requiring research support.

Fischer-Tropsch Synthesis

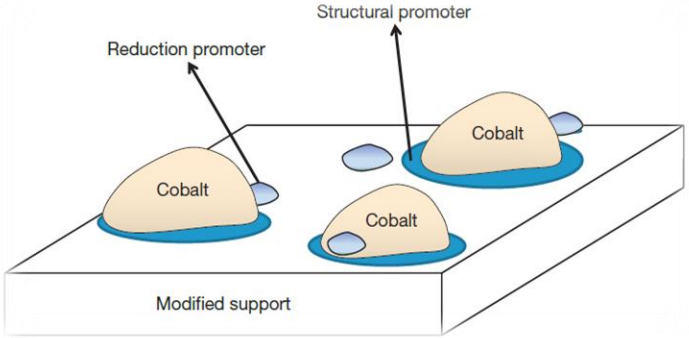
Prof. Franz Fischer

Dr. Hans Tropsch





Hydrocarbon product spectrum for various chain growth probabilities.
0.70 < α < 0.75 HTFT
0.85 < α < 0.95 LTFT



Cobalt catalyst schematic composition

$$FTS: CO + 2H_2 \rightarrow -CH_2- + H_2O \quad (-165\frac{kJ}{mol})$$

$$WGS: CO + H_2O \leftrightarrow H_2 + CO_2 \quad (-42\frac{kJ}{mol})$$

www.sasol.com
http://www.mn.uio.no/ingap/english/research/projects/fischer-tropsch/
http://www.tc2.ch.tum.de/fileadmin/tuchtc2/www/ICP1/ICP1_1314/9-FT_synthesis-2013_PW.pdf

van de Loosdrecht J., et al, Fischer–Tropsch Synthesis: Catalysts and Chemistry. In: J. Reedijk and K. Poeppelmeier, ed. Comprehensive Inorganic Chemistry II, Vol 7. Oxford: Elsevier; 2013. p. 525-557.

Ingredient 6: Challenging research questions.

Crystalline phase ↔ catalyst activity

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Article outline

Abstract
References

Applied Catalysis

Volume 16, Issue 2, 15 May 1985, Pages 215–225

ELSEVIER

Iron/manganese oxide catalysts for Fischer-Tropsch synthesis. Part II: Crystal phase composition, activity and selectivity

G.C. Maiti, R. Malessa, U. Löchner, H. Papp, M. Baerns

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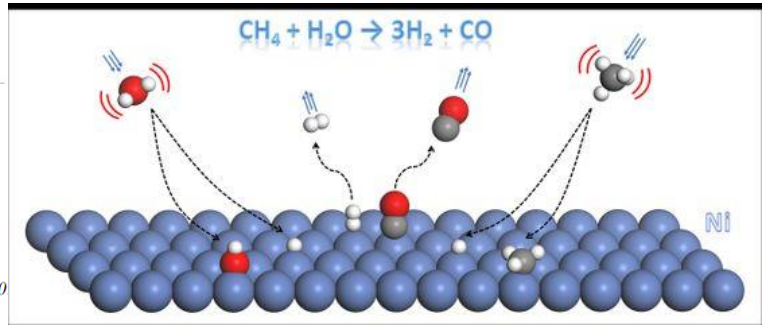
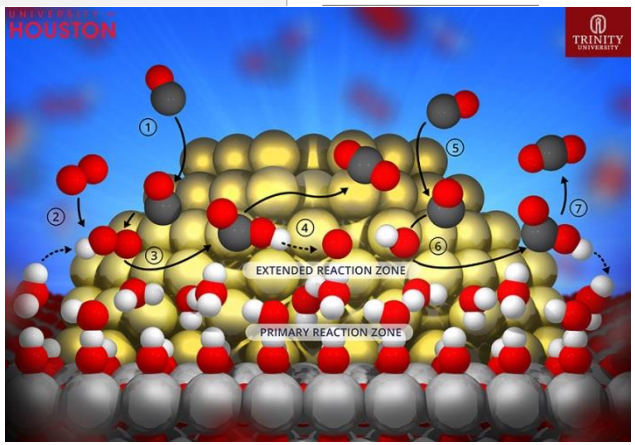
Catalysis Letters Vol. 82, No. 3–4, October 2002 (©200

DOI: 10.1016/S0166-9834(00)84





Fischer–Tropsch synthesis: changes in phase and activity during use

Nathila Sirimanothan [a], Hussein H. Hamdeh [b,*], Yongqing Zhang [a], and Burtron H. Davis [a]

[a] *University of Kentucky, Center for Applied Energy Research, 2540 Research Park Drive, Lexington, KY 40511, USA*
[b] *Wichita State University, Physics Department, Box 32, Wichita, KS 67260, USA*

Received 5 September 2001; accepted 8 May 2002

Four iron catalysts (unpromoted, K-promoted, Si-promoted and K,Si-promoted) were activated and subjected to common Fischer–Tropsch synthesis conditions. At increasing times on stream, samples were withdrawn from the continuously stirred tank reactor in the reactor wax while keeping the sample blanketed with an inert gas. Mössbauer spectra were recorded for various samples and the iron phases of the catalyst were compared to the catalytic activity. A simple model based on bulk composition of the catalyst is not related to the catalytic activity during the course of the run.

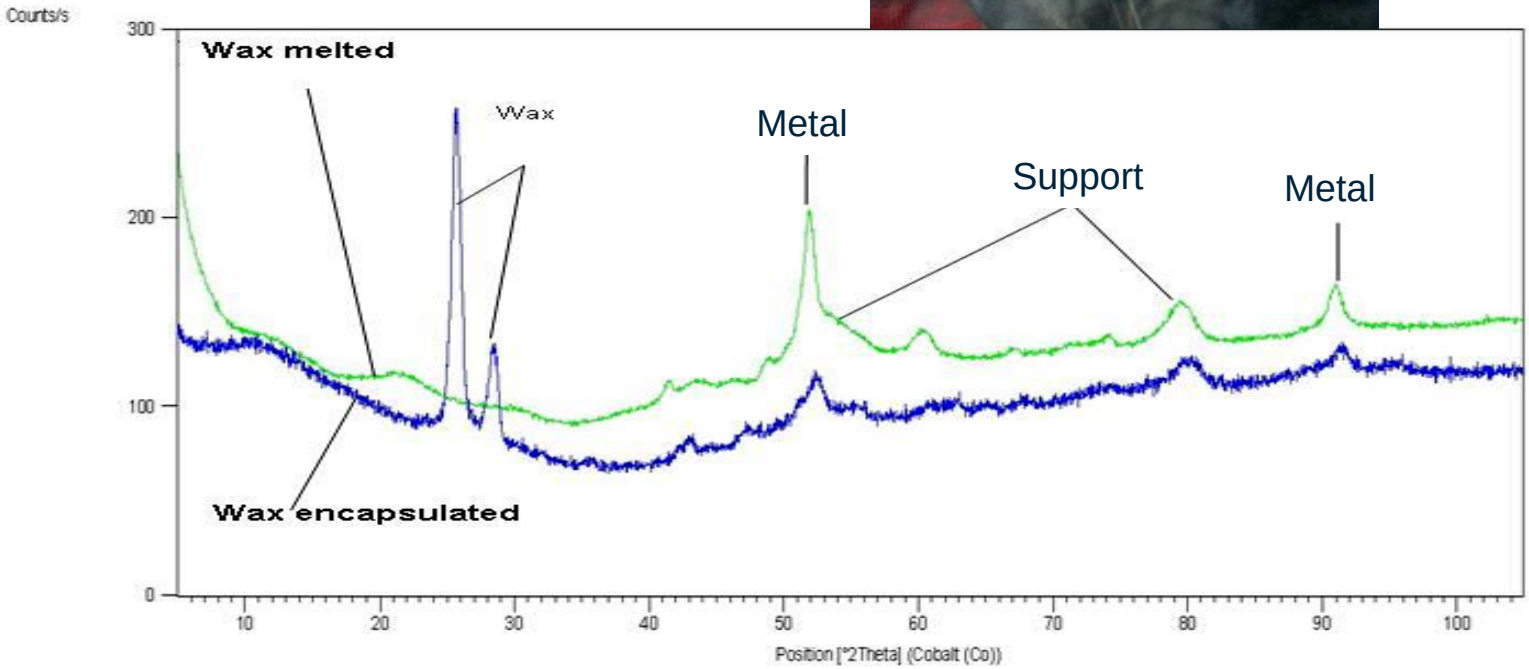
KEY WORDS: Fischer–Tropsch synthesis; iron catalyst; Mössbauer studies of iron.

http://new.trinity.edu/news/science-publishes-trinity-chemistry-research-results

Ingredient 6: Challenging research questions.

Wax coated catalyst:

- Small crystallites (2 – 50 nm)
- Mixture of phases
- In situ studies

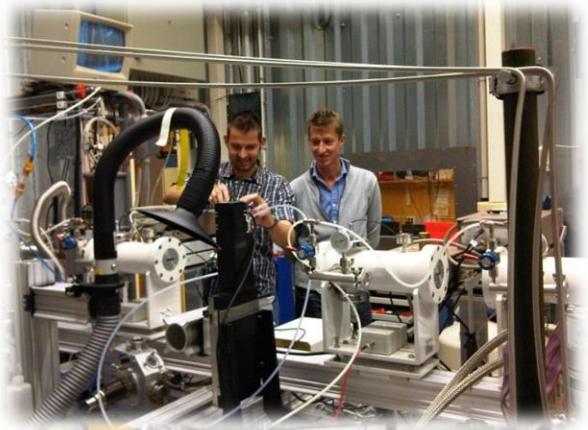


Poster: Catsa 2007, B. Breedt, *et al*

Ingredient 7: A solid home base.

Characterization expertise in Analytics

Technique	Equipment	Technique specialist
XRD & synchrotron	*2 Panalytical X'Pert Pro MPD, 1 Empyrean Panalytical XRD* *In situ reactors XRK600, XRK900, 2x HTK2000, capillary* *Bruker D8 with Co and Mo-radiation* *HR XRD & PDF, EXAFS/XANES*	Esna du Plessis Marietjie du Toit Ghislaine ter Stege Ben Ashton



Ingredient 7: A solid home base – Corporate Governance

Sasol Group Technology makes use of synchrotron & neutron techniques.

Cutting edge analytical techniques.

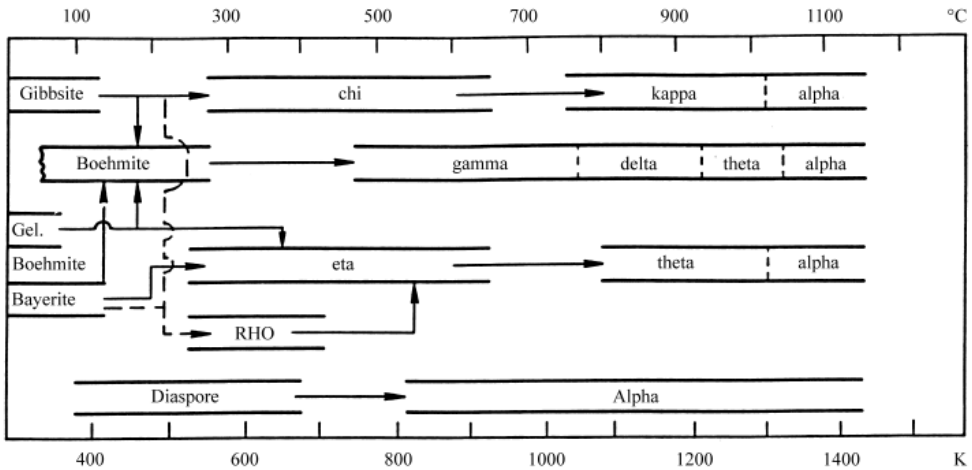
Fits into our analytical portfolio.

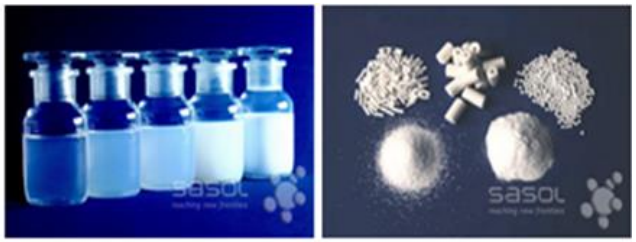
Corporate governance guides process to purchase commercial beam time.

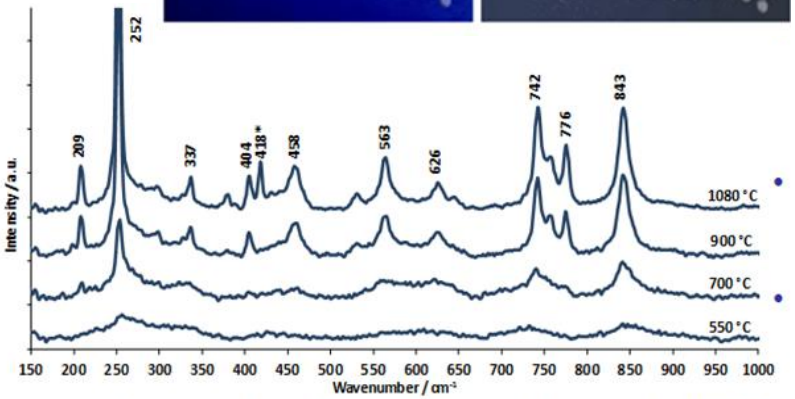
Encourage post graduate students to make use of synchrotron and neutron opportunities.

Ingredient 8: Prove synchrotron & neutron applications.

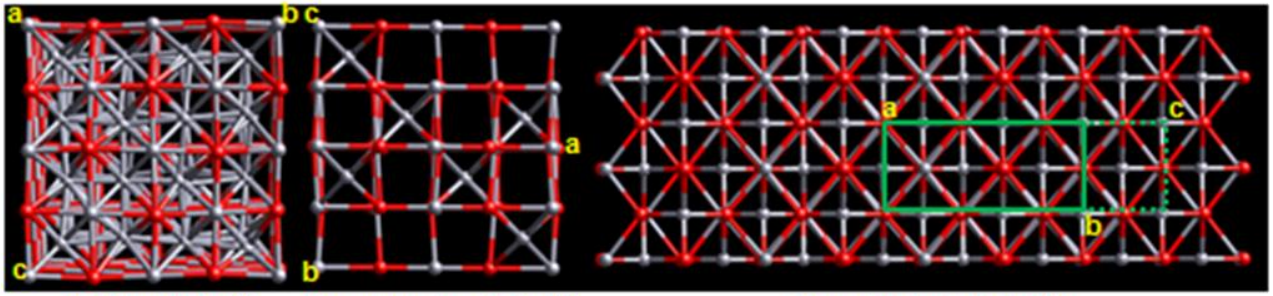
Crystal structure of "δ-Al_2O_3"







Raman spectra of the a γ-Al_2O_3 catalyst support calcined at increasing temperature.



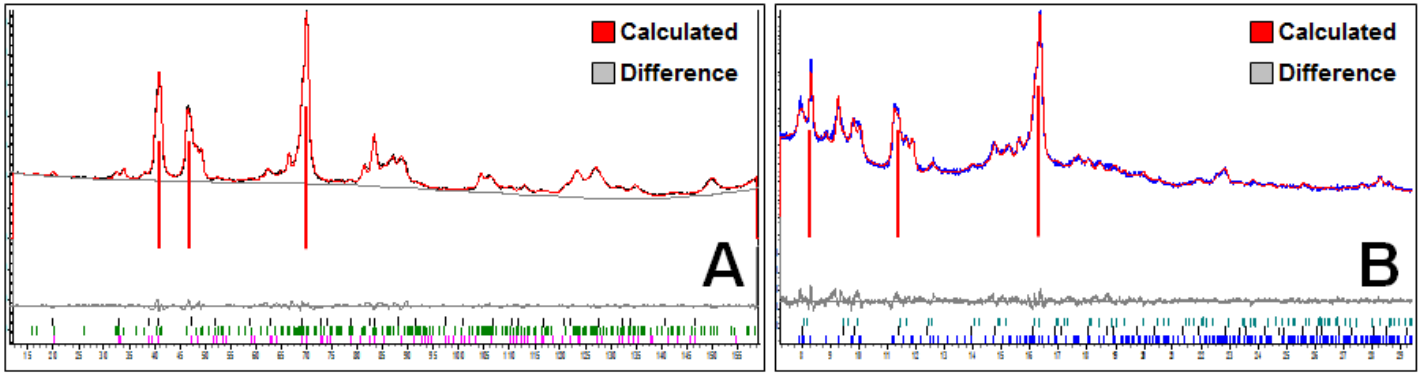
Cubic γ-Al_2O_3[9] **Tetragonal γ-Al_2O_3[10]** **Monoclinic θ-Al_2O_3[11]**

The formation of α-Al_2O_3 is evidenced by 418 cm^{-1} band. Figure shows a disordered θ-Al_2O_3 surface phase at 550 °C, ordering with temperature increase

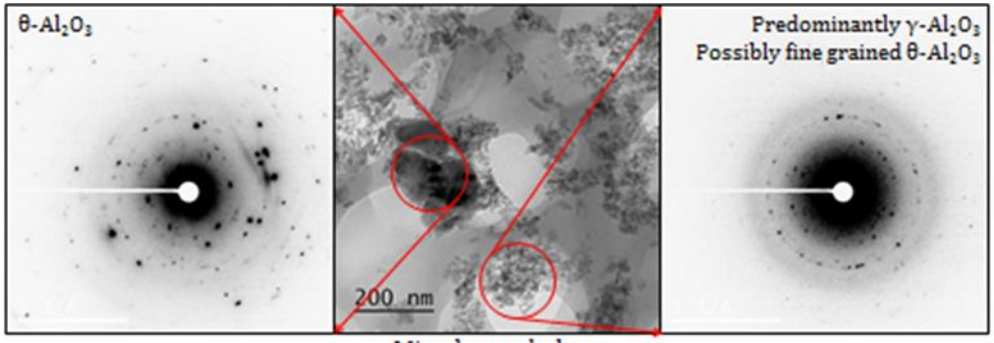
Wefers K, Misra C. *Oxides and hydroxides of aluminium*, **1987**, ALCOA Laboratories, Pennsylvania, USA, p. 20.
Kim H, Kosuda KM, Van Duyne RP, Stair PC. *Chem. Soc. Rev.*, **2010**, *39*, 4820-4844.
Smrčok Ľ, Langer V, Křesťan J. *Acta Cryst.*, **2006**, *C62*, i83-i84.
Paglia G, Buckley CE, Udovic TJ, Rohl AL, Jones F, Maitland CF, Connolly J. *Chem. Mater.* **2004**, *16*, 1914-1923.
Yamaguchi G, Yasui I, Cmu WC. *Bull. Chem. Soc. Jpn.*, **1970**, *43*, 2487.

Ingredient 8: Prove synchrotron & neutron applications.

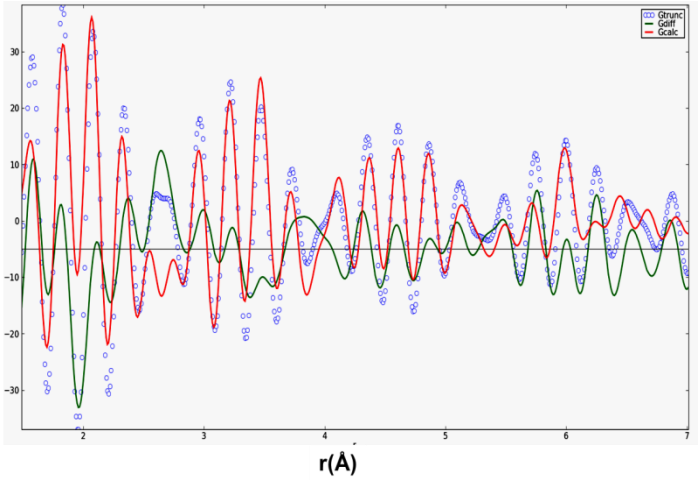
δ-Al_2O_3 = γ-Al_2O_3 + θ-Al_2O_3



Match of theoretical and experimental diffractograms for (A) Neutron °2θ, λ=1.00Å and (B) Synchrotron X-rays °2θ, λ=0.40Å (| reflections originating from oxygen lattice).



Mixed morphology
Fine & coarse



PDF refinement of δ-Al_2O_3 sample

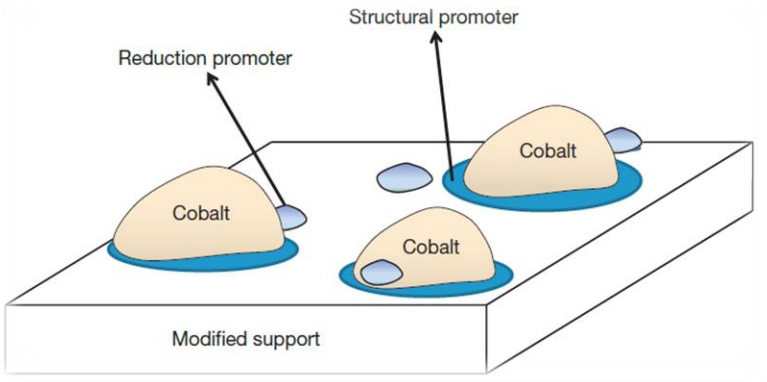
Ingredient 9: Continuous implementation of synchrotron gained knowledge.

Powder XRD for catalyst characterization

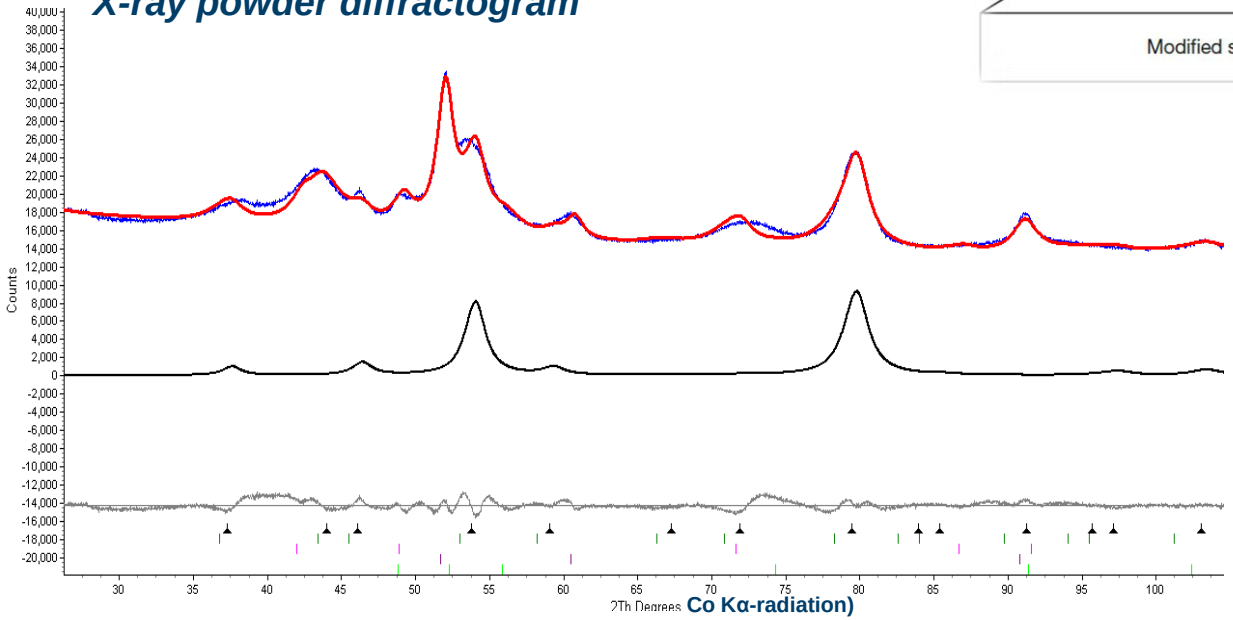
Quantitative phase analysis:

Topas5 routinely applied to 60 – 100 samples per month

In situ XRD



X-ray powder diffractogram



Experimental diffractogram (blue)
Theoretical diffractogram (red)

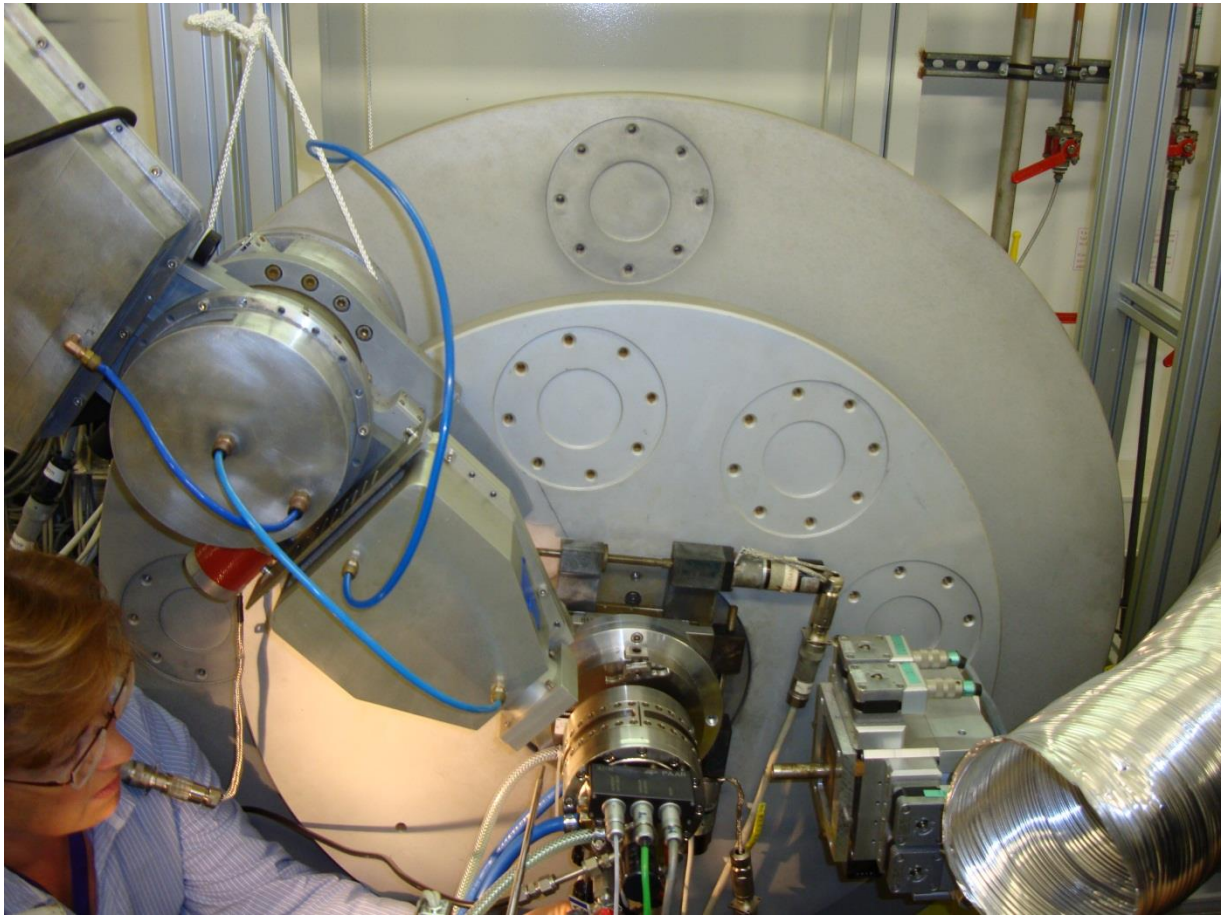
Theoretical diffractogram of support

Difference diffractogram

Relative abundances of crystalline phases
Average crystallite sizes of crystalline phases

Ingredient 10: Grow synchrotron knowledge.

In situ high resolution XRD experiment



ID31 31 keV

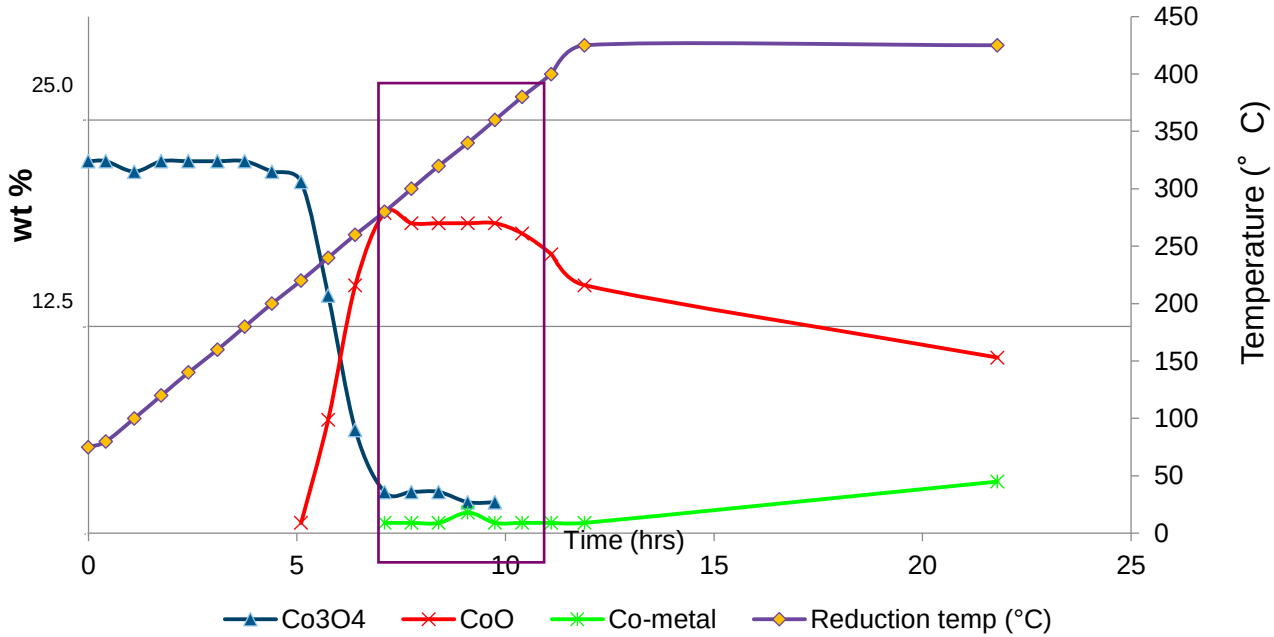
Anton Paar XRK900

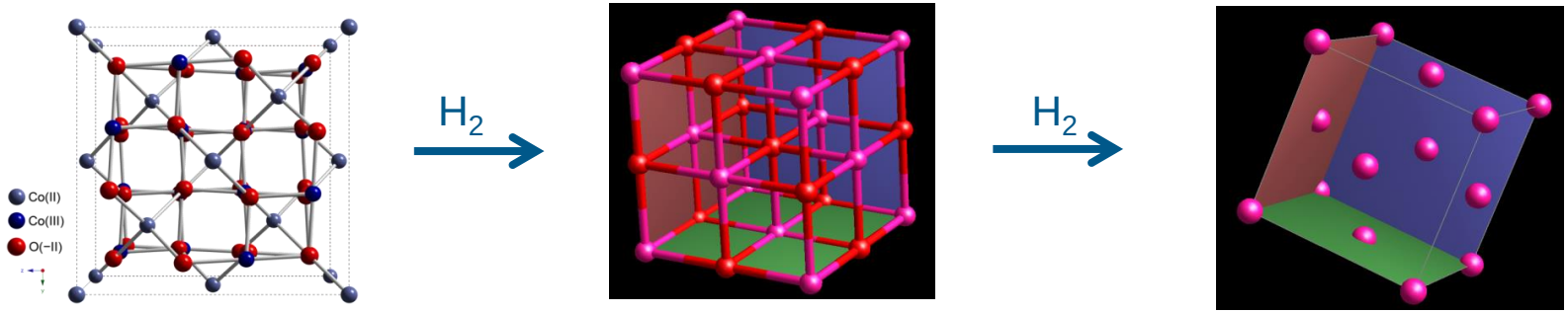
H_2

80 → 425 ° C

Ingredient 10: Grow synchrotron knowledge.

Reduction of Co/alumina model catalyst (no promoters)





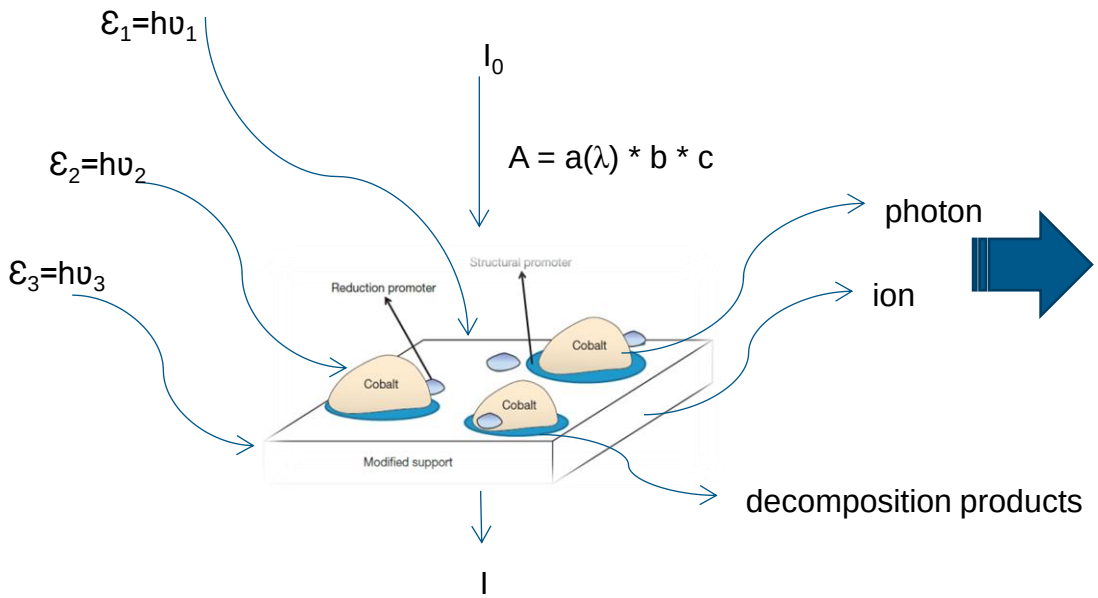
du Plessis, H.E.; Forbes, R.P.; Barnard, W.; Erasmus, W.J.; Steuwer, A. *Physical Chemistry Chemical Physics*, 2013, 11640-11645.

Ingredient 11: Advance Intellectual Property

Key outputs

	2015	2014	2013
Number of new patents added	**30**	65	135
Investment in research and development	**R1 645m**	R1 550m	R1 433m
Investment in bursary scheme	**R40,3m**	R47,0m	R54,7m
Undergraduate and postgraduate bursars	**440**	577	719
Investment in South African universities	**R16m**	R15m	R25m
Number of workplace/leadership coaches mentored	**122**	393	257
Intangible assets	**R1,7bn**	R1,9bn	R1,4bn

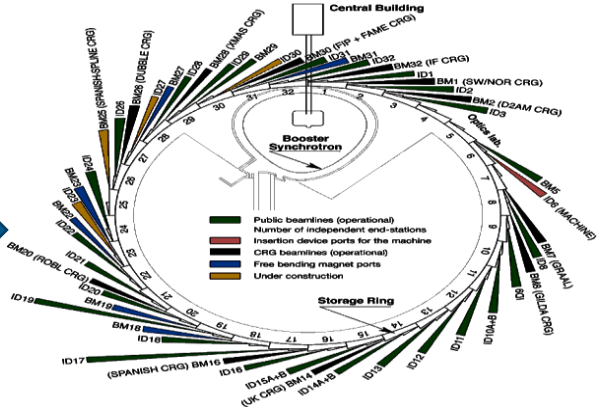
Final ingredient: Compose an analytical symphony..



Relevance of research at synchrotrons for African Industries

Ingredients	Africa
Sustainable value creation	Inputs & outputs – optimize?
Leverage international footprint	Networks – grow
Developing people	√ - momentum
Enhancing stakeholder relationships	√ - momentum
Technologies requiring research support	Clean water, palaeontology, Ebola
Challenging research questions	Nano-technology for clean water, drug design, drug delivery design
A solid home base	Grow
Prove synchrotron & neutron applications	Celebrate victories
Continuous implementation of synchrotron gained knowledge	Feedback loop
Grow synchrotron knowledge	Partner countries, access, review, synchrotron schools
Advance Intellectual Property	Publications and peer reviewed output
Compose an AFRICAN symphony	YES

Compose an African synchrotron symphony!



Thank you

- African Light Source conference & workshop organizing committee
- Sasol Group Technology
- South African Institute of Physics
- SA synchrotron committee members

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