# The role of Plasma Modelling in Industrial Research

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Quantemol

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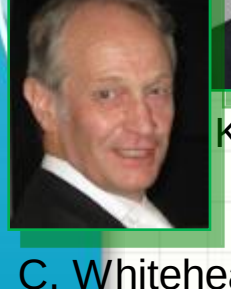
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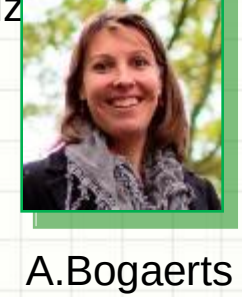
A.Bogaerts


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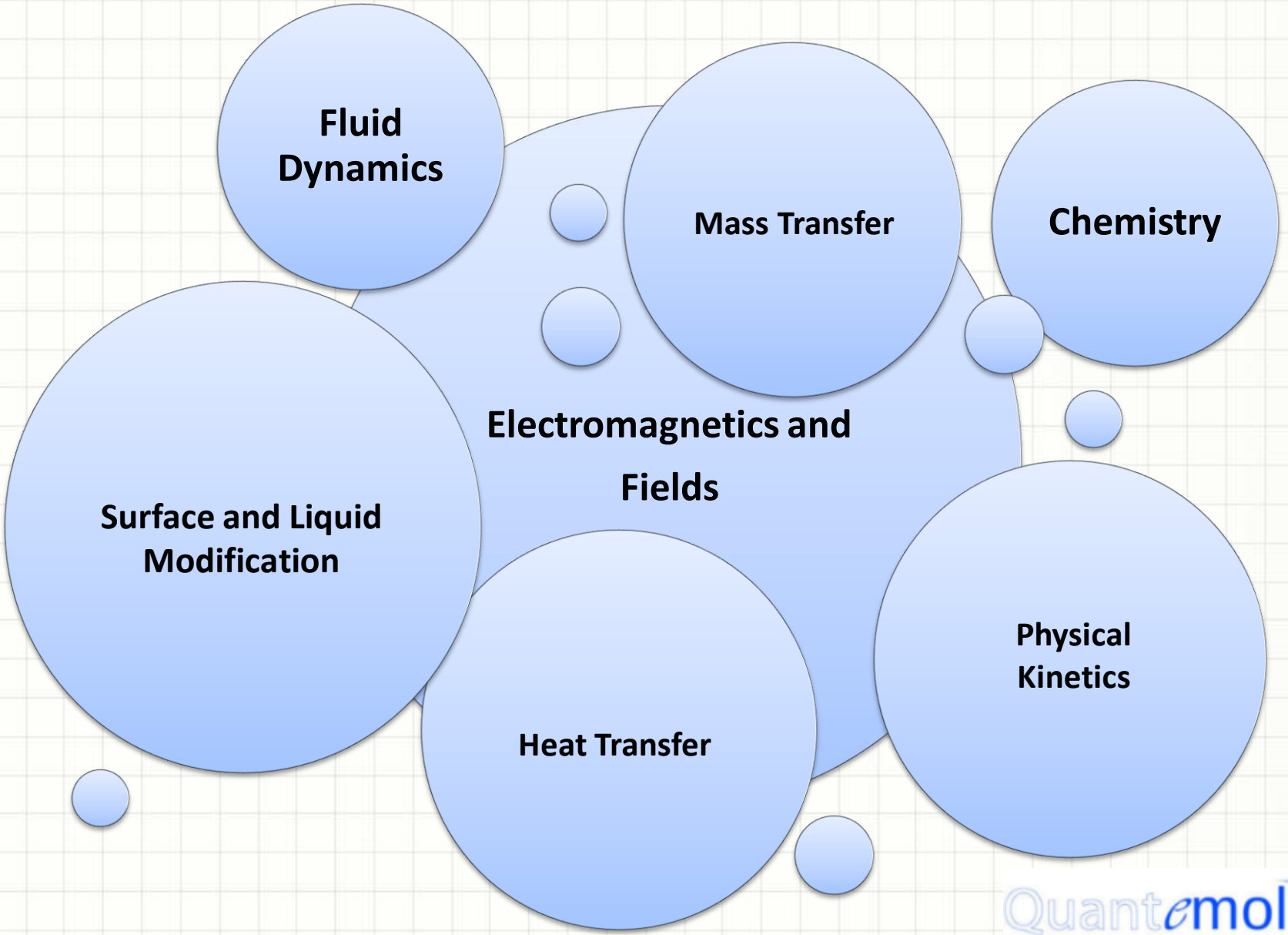
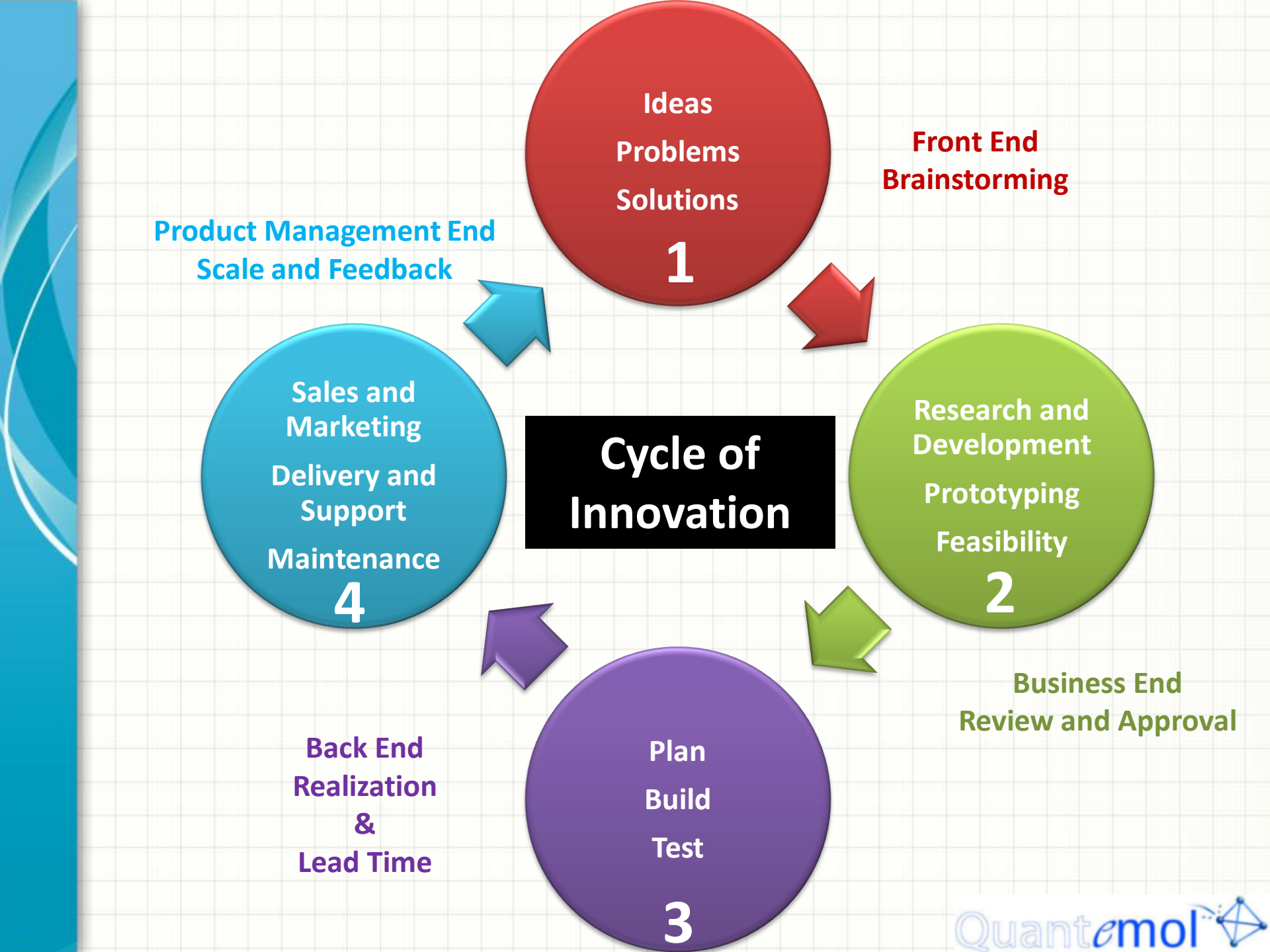
# Low Temperature Plasmas



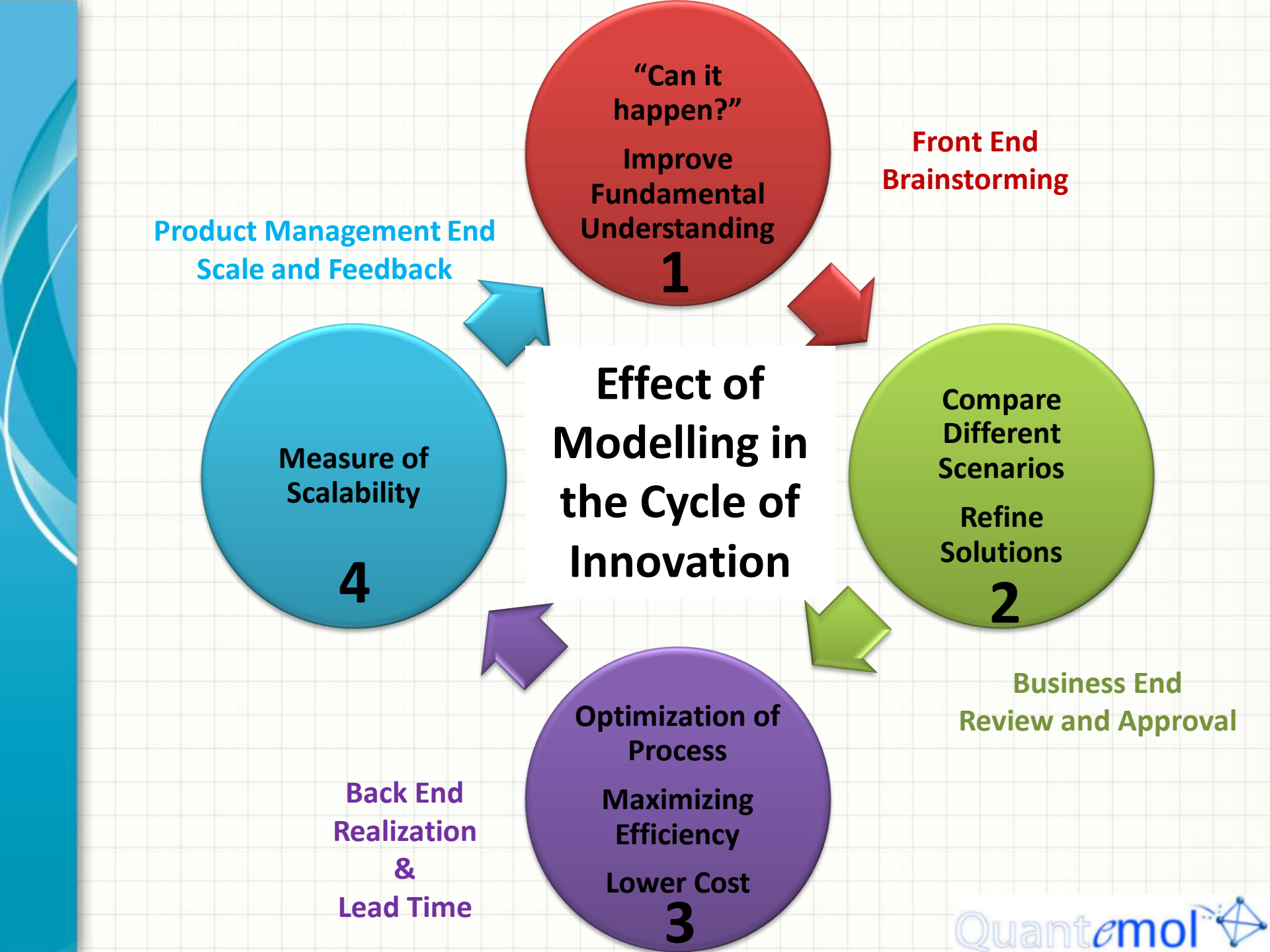
# Interdisciplinary Nature

- Applications in multiple industries
- Wide scope for academic research
- No current limitation on application
  - Critical feature down to single nm
  - Wound cleaning and healing in Biomedicine
  - Agriculture for cleaning crops
  - Gas Abatement
  - Catalysis and Reformation
  - Surface modification and adhesion
- A lot of innovation and progression across multiple industries…

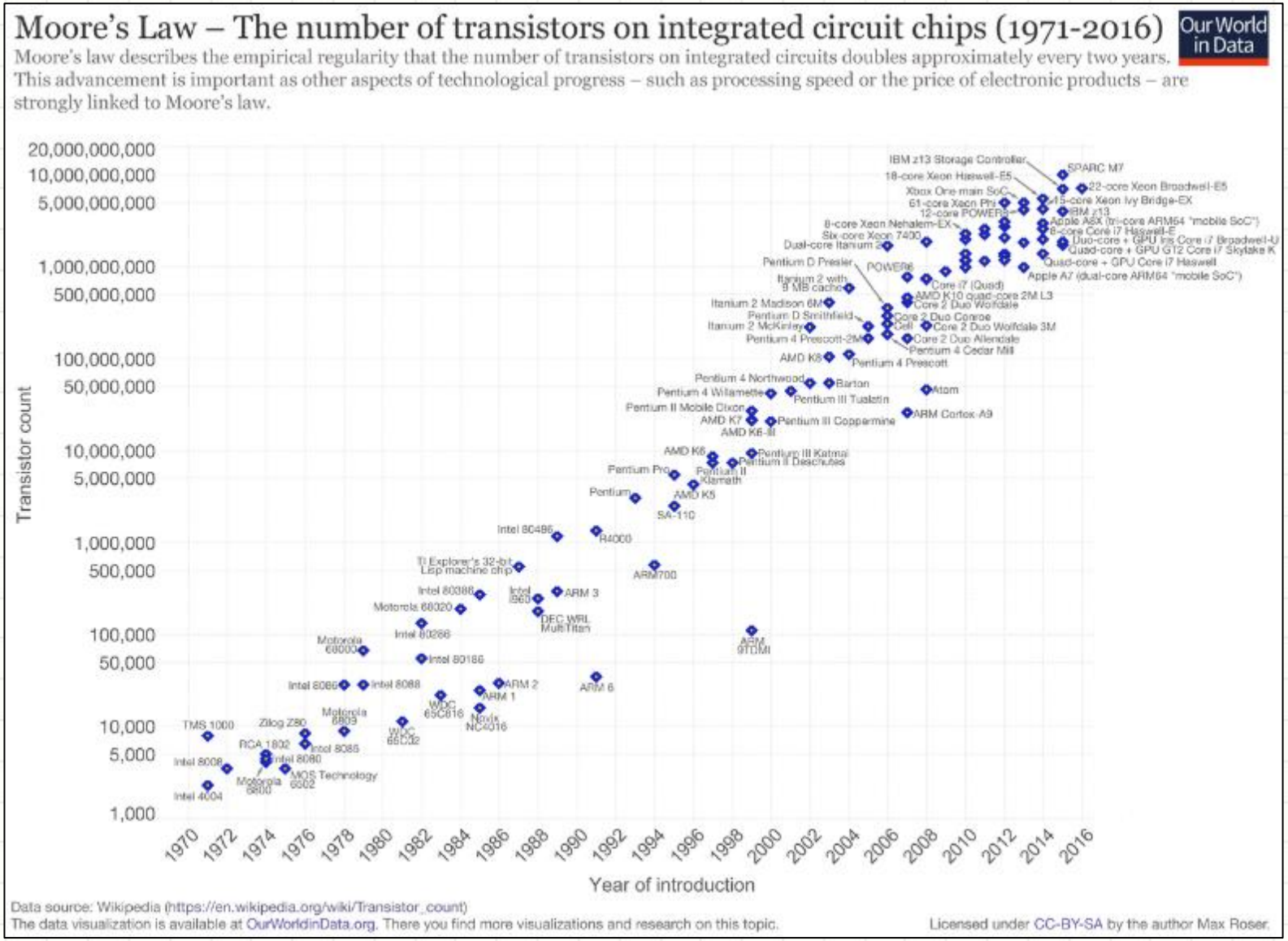

Ideas
Problems
Solutions
1
Front End
Brainstorming
Research and Development
Prototyping
Feasibility
2
Business End
Review and Approval
Plan
Build
Test
3
Back End
Realization
&
Lead Time
Sales and Marketing
Delivery and Support
Maintenance
4
Product Management End
Scale and Feedback
Cycle of Innovation

# Why Model?

- Modelling is essential in order to relate what happens in the plasma/source to the final product
- Gives the ability to make bold predictions backed by fundamentals
- Enables process optimization
- Presents a ‘workspace’ to investigate unforseen or lesser known phenomena
- **An important intermediary when experimentation or repeat prototyping is not practical**
- Relatively cost-effective to carry out
- Saves a lot of **time**
- Prototyping continuously makes optimization effectively impossible. Modelling = tighter feedback loop.


"Can it happen?"
Improve Fundamental Understanding
1
Front End Brainstorming
Compare Different Scenarios
Refine Solutions
2
Business End Review and Approval
Optimization of Process
Maximizing Efficiency
Lower Cost
3
Back End Realization & Lead Time
Measure of Scalability
4
Product Management End Scale and Feedback
Effect of Modelling in the Cycle of Innovation

# Semi-Conductor Fabrication



Transistor count increase coincides with downscaling of feature size

Downscaling of feature size is strongly linked to devices becoming more portable and ergonomic

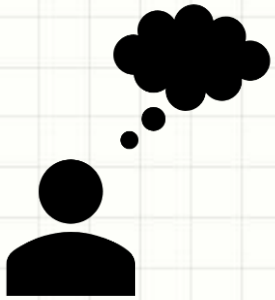
Electronics become more functional and enable the progression of new ideas such as IoT

MOSFET downscaling becomes complicated at 10s/1s of nanometre

There are many physical challenges approaching the fabrication of stable, anisotropic features

Price of electronics has risen because **manufacturing costs have risen**

There needs to be a greater understanding of the physical concepts and processes that occur.



Costs have increased due to more expensive processing tools and upgrades. These have lengthy lead times.

**General understanding of these tools is still not very high**

**Problems**

- Last major node ~ 14 nm (common)
- **Node scaling is expensive – tool and process design very lengthy and costly**
- Growing disconnect between node design and manufacturing

This can be offset through computational techniques

Modelling allows for cheap, time efficient and collaborative investigation into new processes:

- Reducing costs of innovation
- Increasing understanding of physical processes
- Optimizing existing processes
- Mitigates risks

**Modelling enables plasma processing of nodes to continue**

**Solutions**

- **Rather than downscaling nodes, migration can be horizontal**
- Applications in technology are heavily dependent on performance
- Modification of current tools is less expensive
- Modification of current processes is less expensive

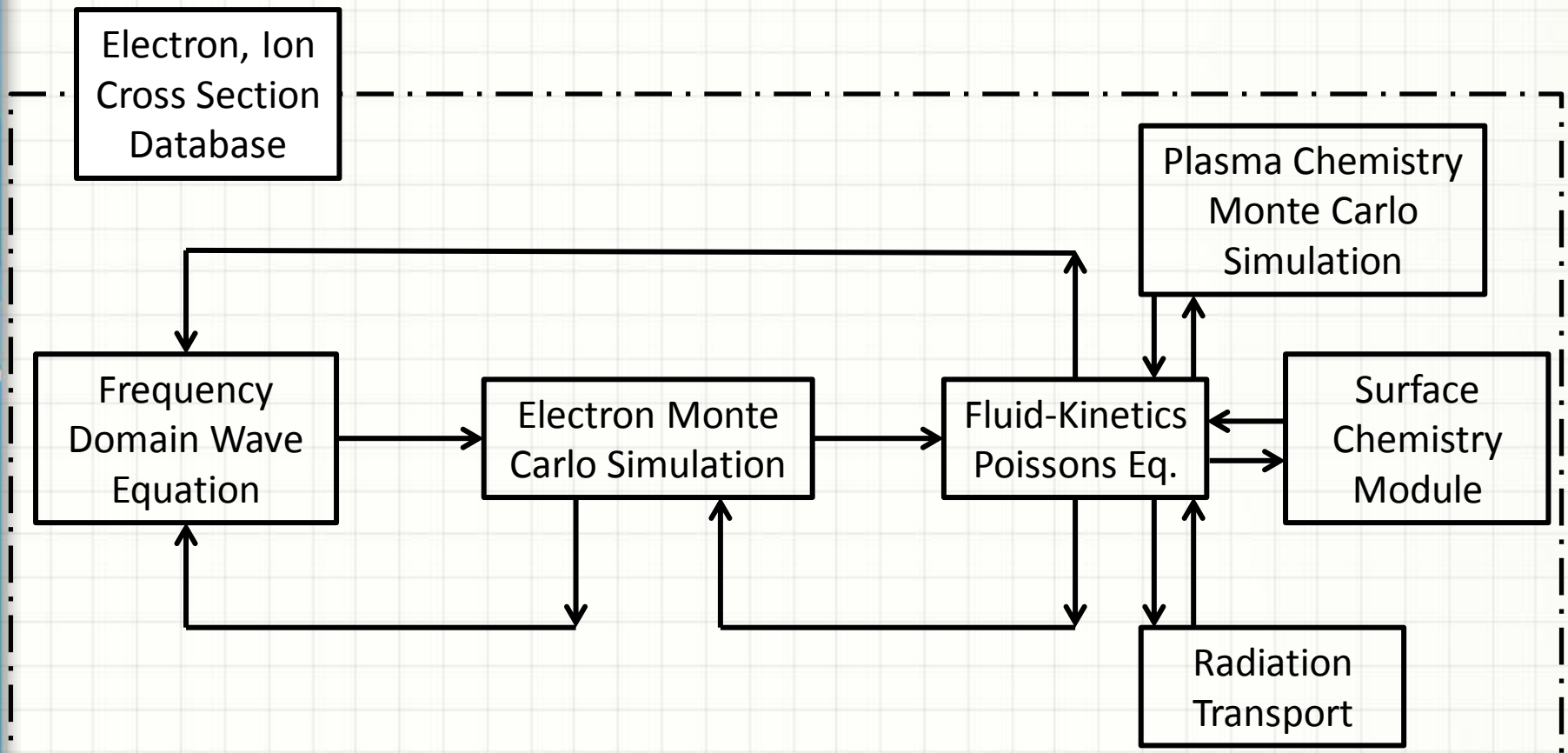
Computational techniques and modelling are the vanguard of implementing new ideas and methods

# Types of Modelling

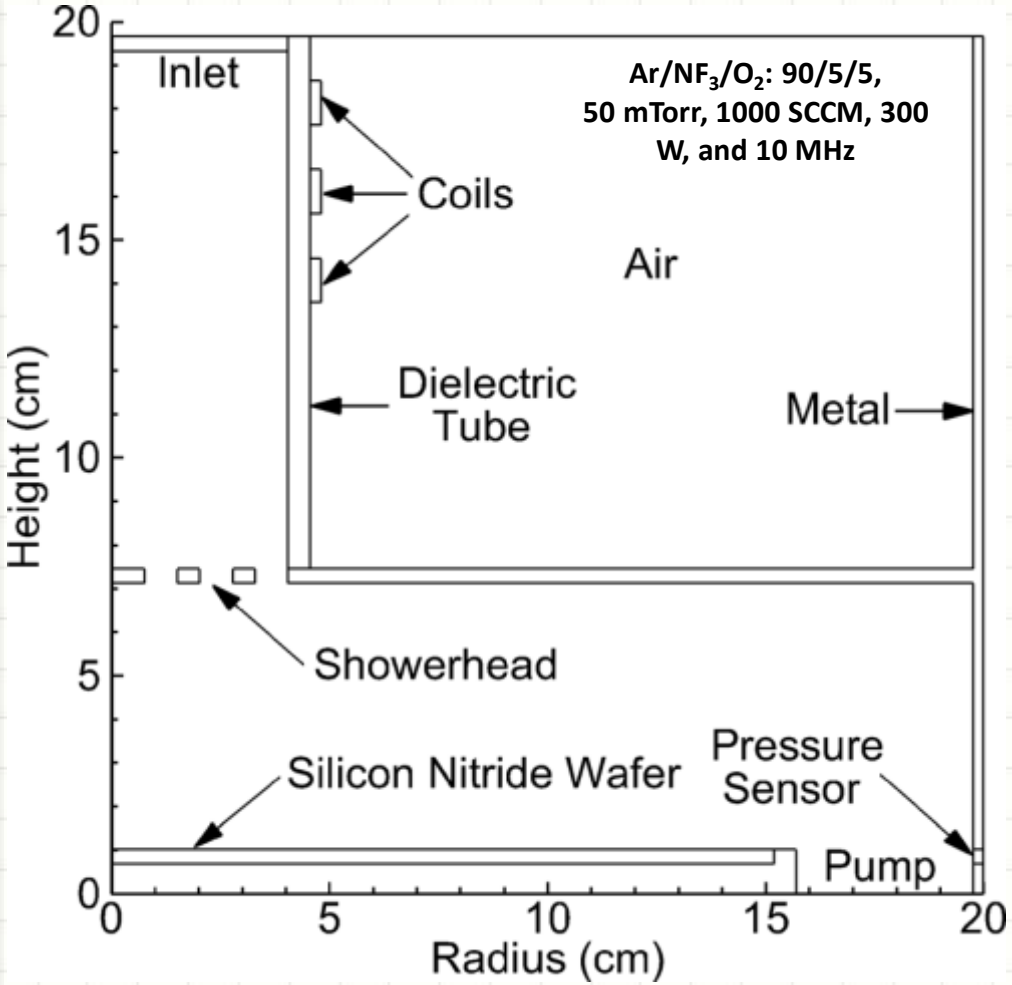
- 0D Modelling
  - Plasma-R
  - Global-kin
  - No geometrical complexity.
  - Cannot investigate reactor behaviours.
  - No set limit to chemistry.
  - Fast computation times
  - Used mainly to study plasma chemistry
- 2D Modelling
  - Q-VT (HPEM)
  - Vizglow
  - Very accurate with 2D symmetrical meshing.
  - Works best with symmetrical reactors.
  - Modular and multiphysical.
  - Depending on the make (QVT), easily computes chemistry and geometry
  - Used for complete tool and process study/optimization
- 3D Modelling
  - COMSOL
  - Opera-D
  - Complex 3D meshing
  - Computationally expensive – multiplied by inputs. Limited to ~ 50 reactions
  - Asymmetric modelling with same modelling performance as 2D but greater time
  - Used mainly to study asymmetric effects and modes

# Case Study - HPEM

The Hybrid Plasma Equipment Module (HPEM)* is the industry standard for describing industrial processing plasmas and tools. It was one of the first computational tools to be developed. **It is distributed as Q-VT**.




* *"Hybrid Modelling of Low Temperature Plasmas for Fundamental Investigations and Equipment Design"*, M. Kushner, 2009, J. Phys. D 42, 194013



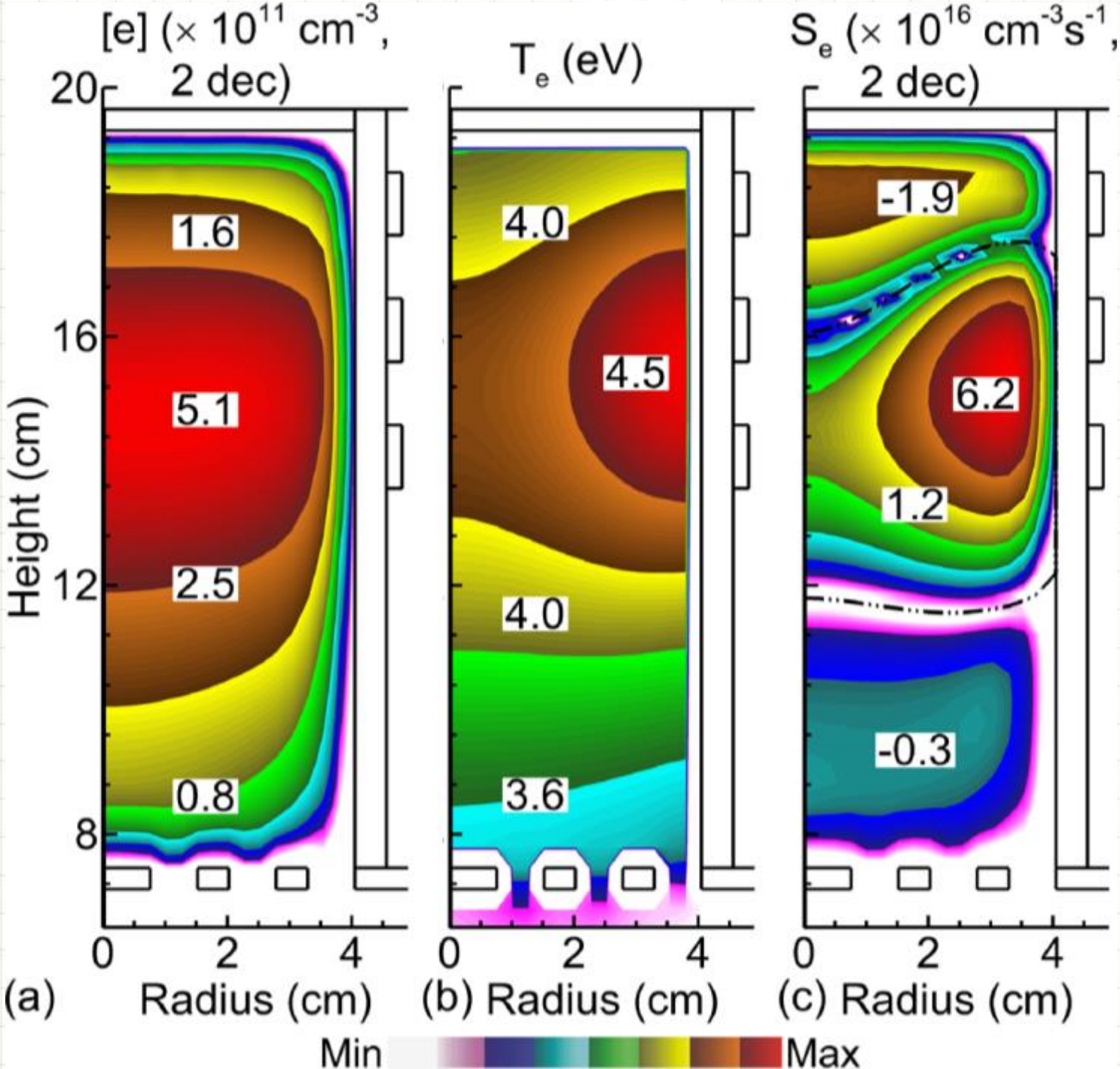

Remote plasma sources:

- Provide passivation
- Provide chemical based etching
- Separated regions of plasma generation and processing
- Reduce/negate the damaging effect of highly energetic ions or UV photons

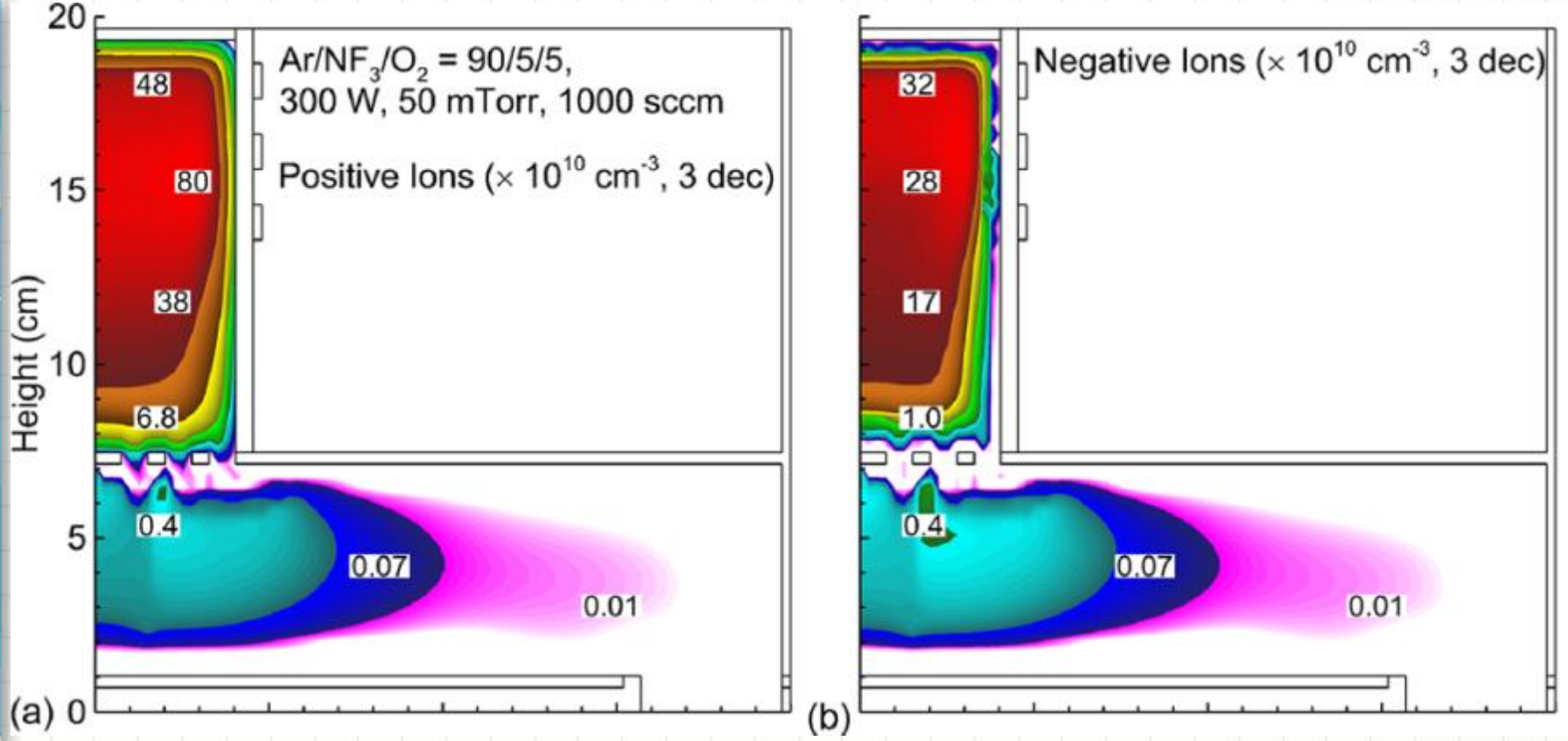
This process seems a little removed from more standard processes. Do we just make it and run it? No!

Use HPEM to recreate the geometry and study the reactor dynamics. Can monitor the flux of important, reactive species to the wafer.

*"Downstream etching of silicon nitride using continuous-wave and pulsed remote plasma sources sustained in $Ar/NF_3/O_2$ mixtures"*, S. Huang & V. Volynets, 2018, J. Vac. Sci. Technol A 36, 021305-1

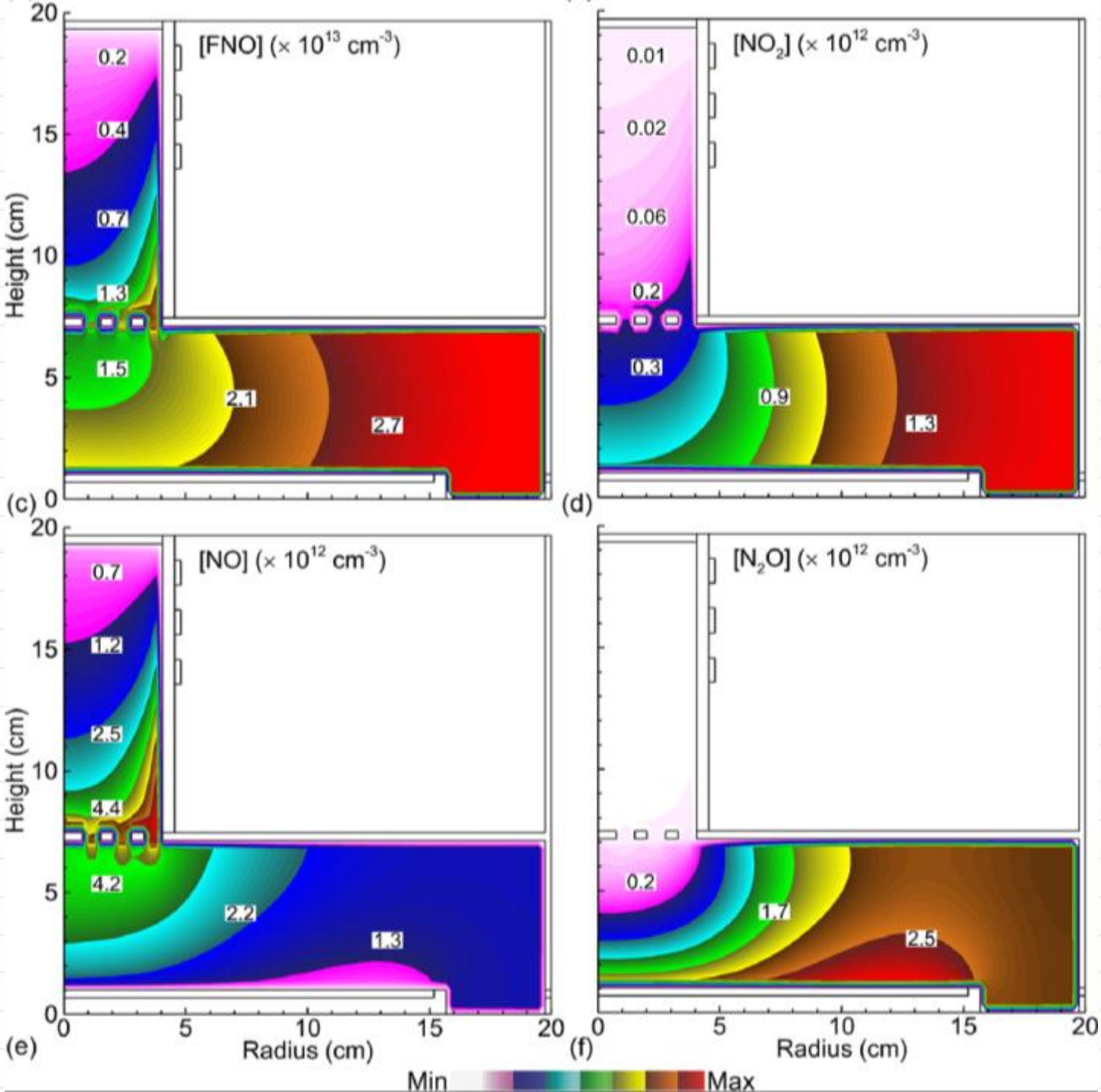

[e] (× 10^11 cm^-3, 2 dec)
T_e (eV)
S_e (× 10^16 cm^-3 s^-1, 2 dec)
Height (cm)
20
16
12
8
1.6
5.1
2.5
0.8
4.0
4.5
4.0
3.6
-1.9
6.2
1.2
-0.3
0
2
4
(a) Radius (cm)
(b) Radius (cm)
(c) Radius (cm)
Min
Max

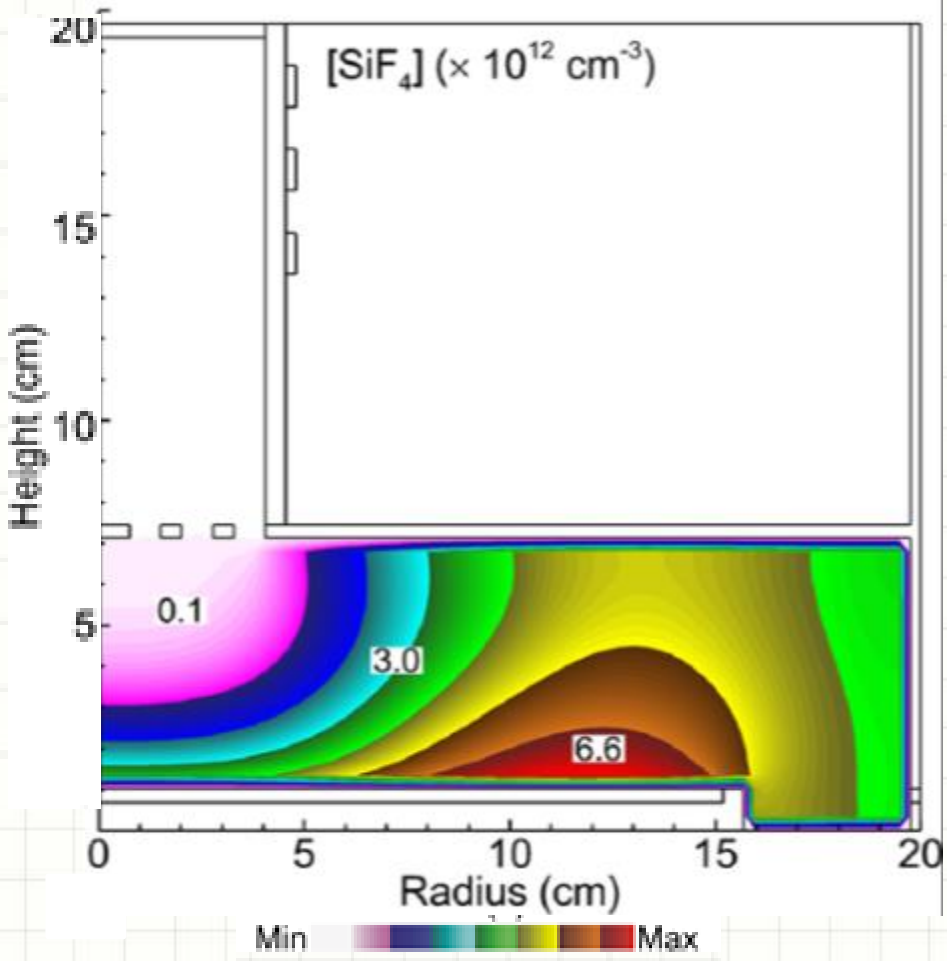
# What happens at the Wafer?




Very low flux of charges to the wafer established.

This isn't just computational 'tinkering', the result obeys real physics.


[FNO] (× 10^13 cm^-3)
0.2
0.4
0.7
1.3
1.5
2.1
2.7
(c)
[NO2] (× 10^12 cm^-3)
0.01
0.02
0.06
0.2
0.3
0.9
1.3
(d)
[NO] (× 10^12 cm^-3)
0.7
1.2
2.5
4.4
4.2
2.2
1.3
(e)
[N2O] (× 10^12 cm^-3)
0.2
1.7
2.5
(f)
Height (cm)
Radius (cm)
0
5
10
15
20
Min
Max




From this result it is reinforced that that main chemical etchant is F radicals.

Any remote plasma process needs to lean on facilitating a flux of diffuse F radicals

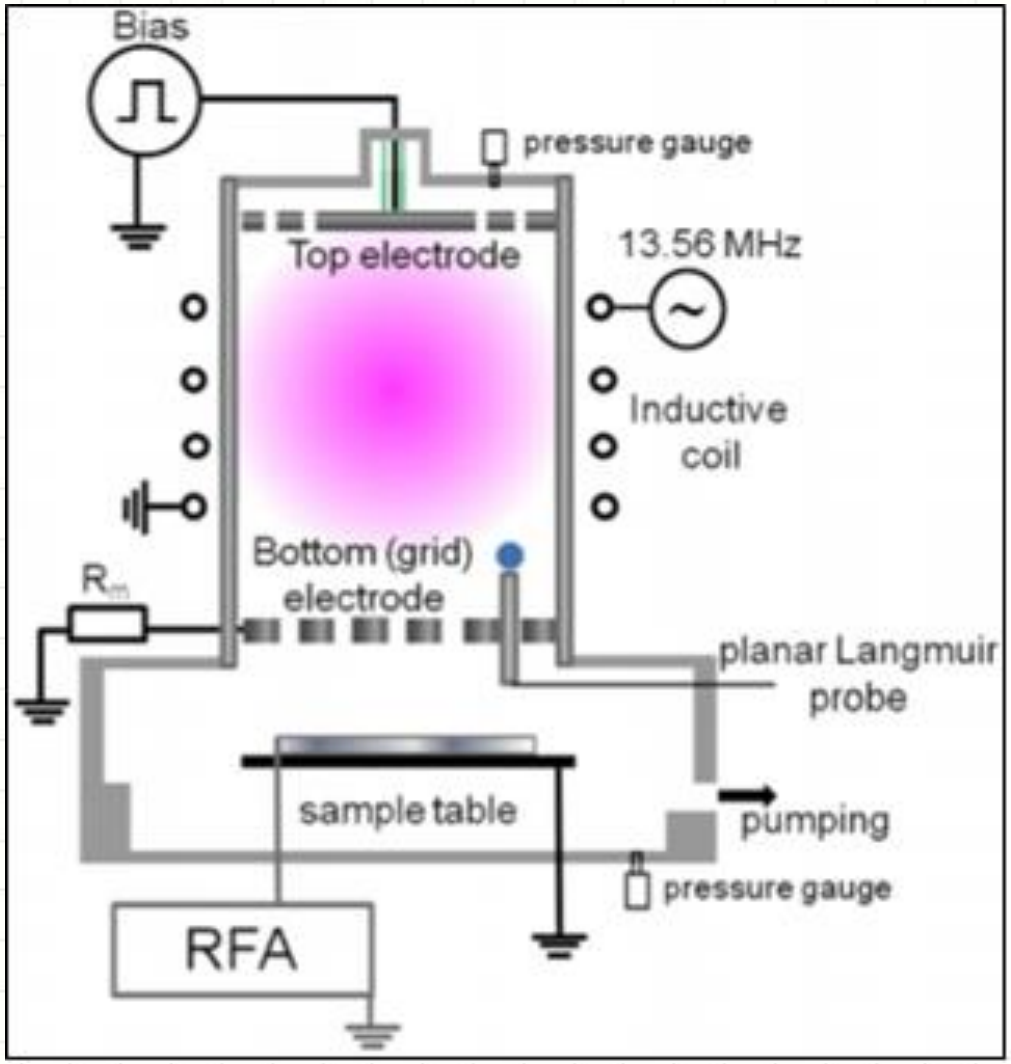
**Fundamental understanding has improved**

**Ideas for process geometries and conditions are more understood**

$Ar/NF_3/O_2$ mixtures have been investigated since at least 1998 for remote plasma sources. However, the **chemistry is complex** and some previous investigations have resorted to mass spectrometry on an already existing geometry*

* *"Silicon etching in $NF_3/O_2$ remote microwave plasmas"*, P. Matsuo & B. Kastenmeier, 1999, J. Vac. Sci. Technol. A 17,

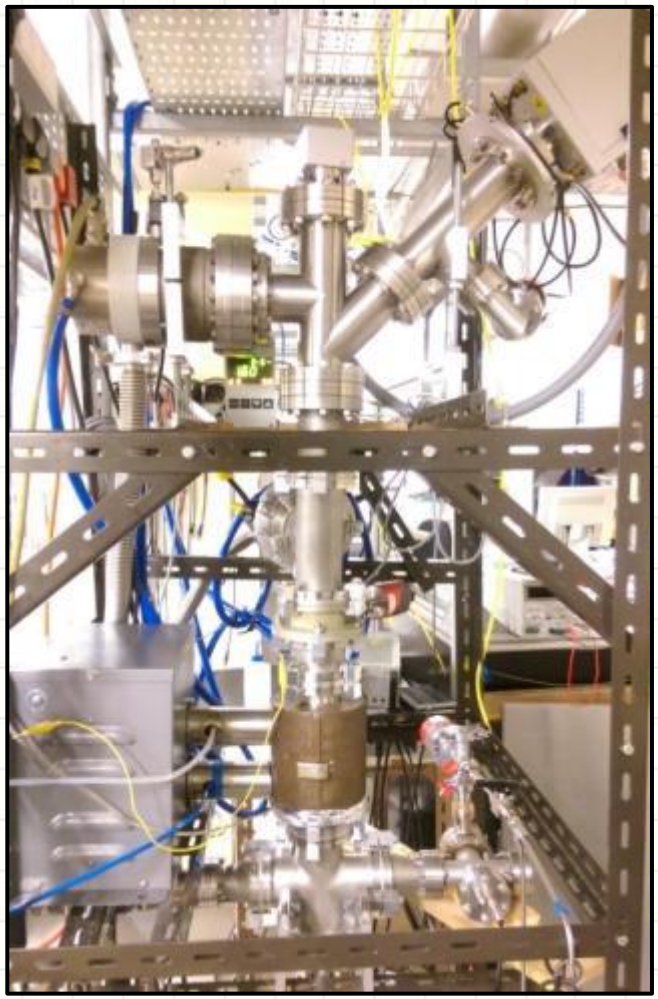
**Not every system/geometry can accommodate such diagnostic methods**

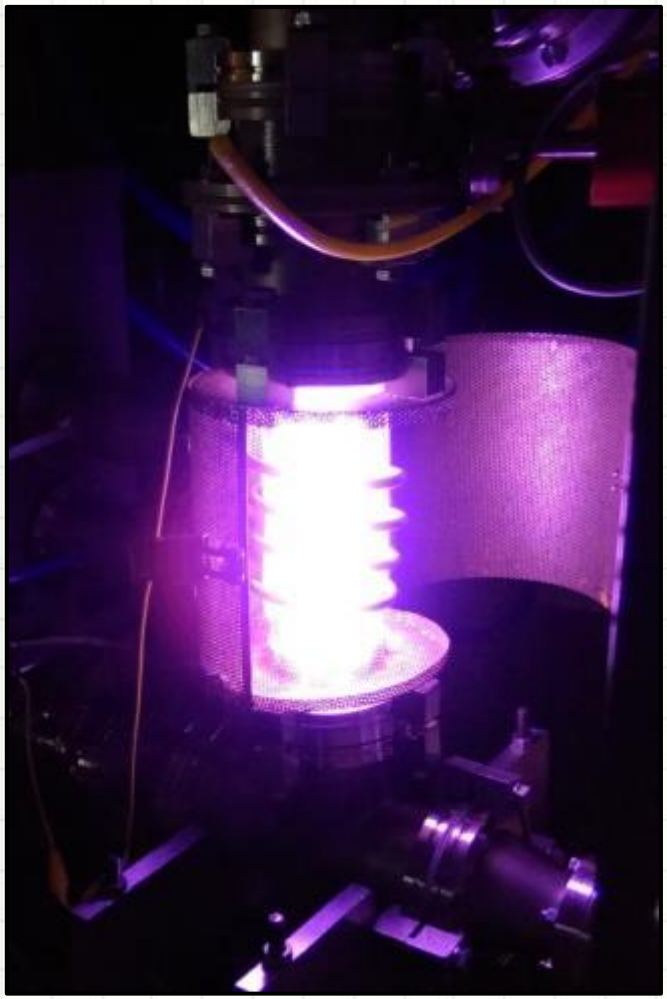



Oxford Instruments PL-80 Plasma Etcher

Discharging mixtures of $SF_6$, Ar and $O_2$ at low pressure (< 30 mTorr) with various powers and flow rates

* *"Extraction and neutralization of positive and negative ions from a pulsed electronegative inductively coupled plasma"."*, D. Marinov & Z. O'Tell, 2015, Plasma Sources Science and Technology, Volume 24, 6





Cost: > £9,000 (Q-VT costs ~ £7,000 with much lower risk!!!)

Lead Time: ~ 2 Years

Time to meaningful/publishable results: ~ 3 years

**For industry, costs are a lot higher and lengthy lead times are unacceptable!!!**

**The chemistry can be modelled and characterized from the ground up**

*This is the subject of the next talk!

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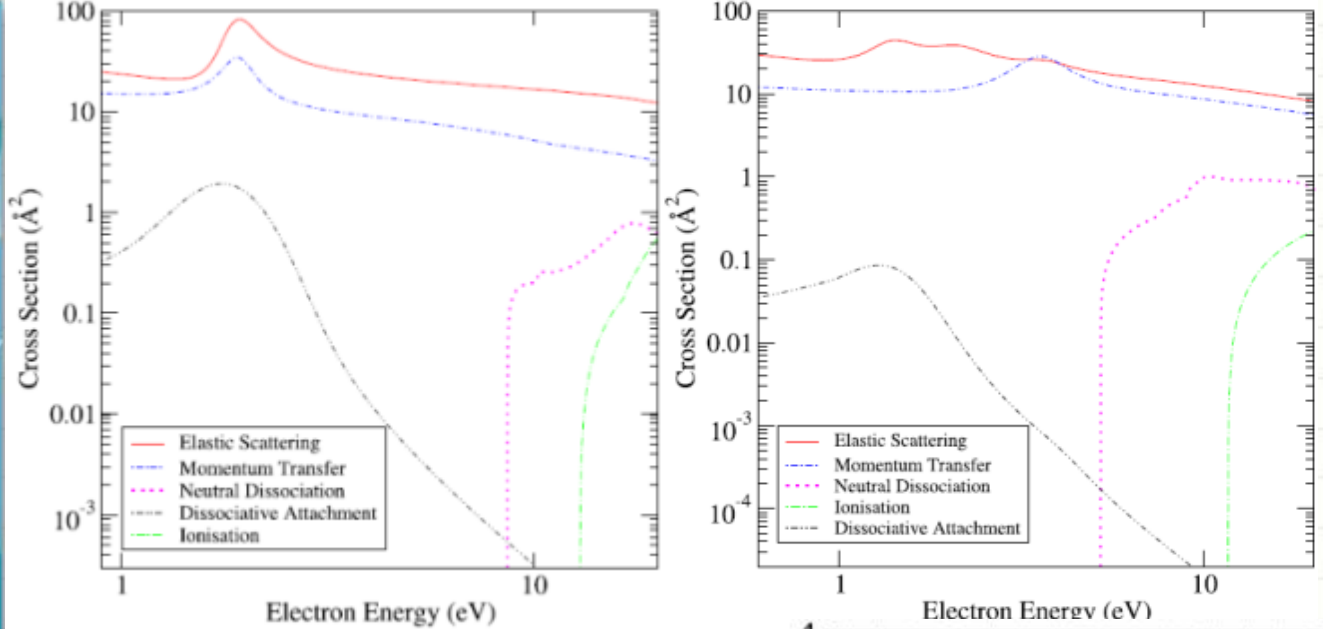
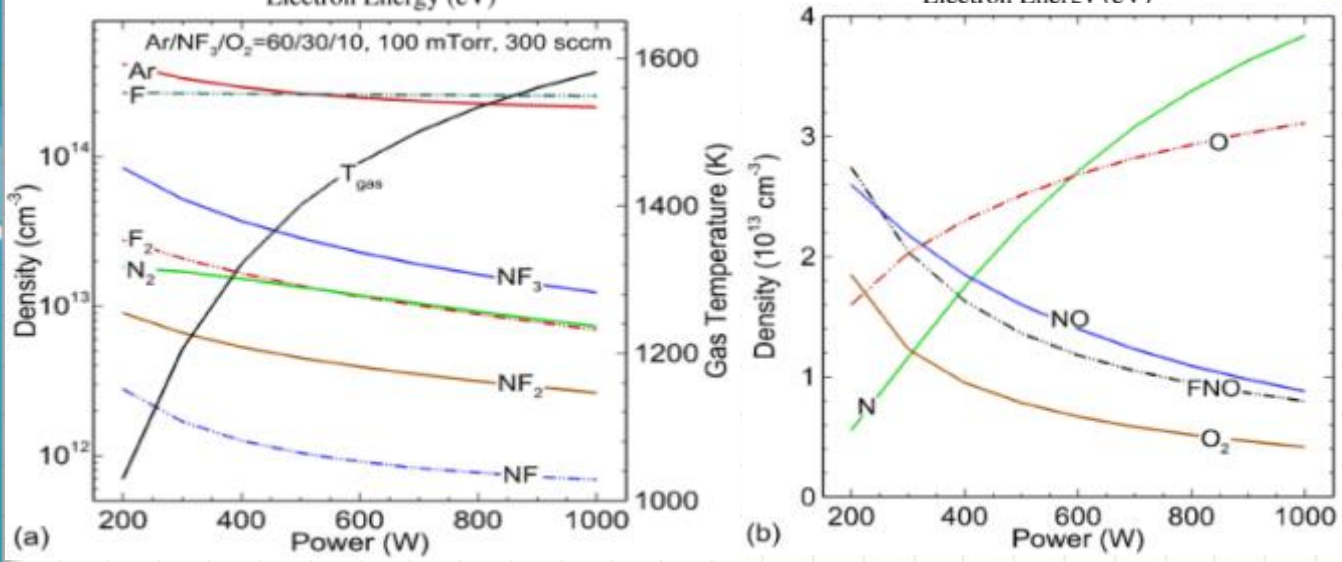



Cross-sections calculated using **Q-N** modelling and R-matrix code




Species density profiles determined using 0D Global-kin modelling.

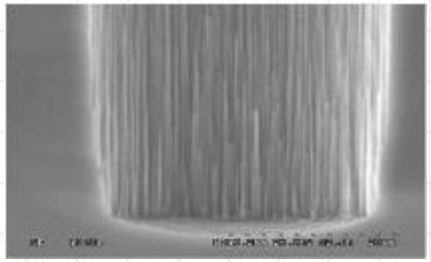
*"Calculated cross sections for electron collisions with $NF_3$, $NF_2$ and NF with applications to remote plasma sources"*, J. Hamilton & J. Tennyson, 2017, Plasma Sources Sci. Technol. 26, 065010

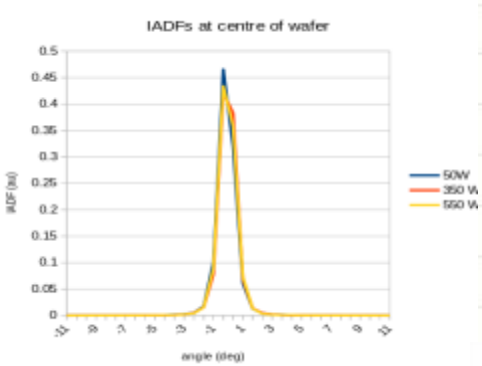
# Modelling of a BOSCH Process

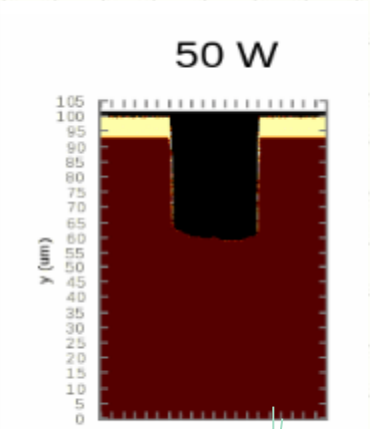
1. **Deposition Step: $C_4F_8$**
2. **Polymer removal Step: $SF_6/O_2$**
3. **Isotropic Chemical Etch Step: $SF_6$**

Data outputted from **Q-VT** was inputted into a Monte Carlo Feature Profile Modeller (MCFPM).

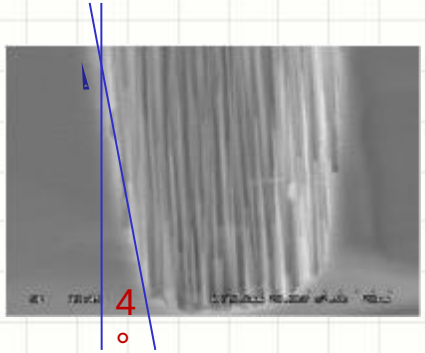
## Middle of the wafer

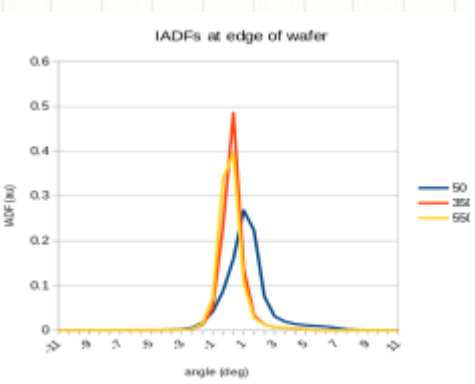


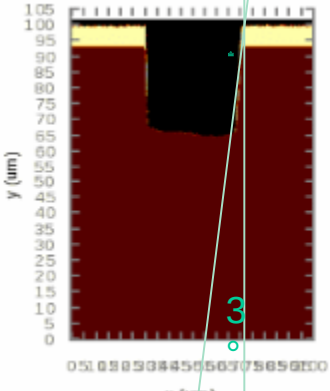



## Edge of the wafer



# Quantemol is involved in the innovation cycle by developing the following tools


**Quantum chemistry code based software to provide cross-sections and reaction rates of both common and exotic species.**


**Modular 2D Plasma modelling software to model plasma behaviour and reactor/tool dynamics.**


**Plasma chemistry database that acts as a repository to store validated plasma chemistries and reactions sets.**

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# Quantemol-VT capabilities: Plasma Dynamics and Reactor Modelling

QVT Virtual Tool

**Geometries and Plasma behaviours which can be investigated using Q-VT:**

- Common geometries such as CCPs, ICPs and Microwave plasmas
- Wide pressure and density range
- Plasma chemistry and species monitoring
- Spatially resolved densities and energy distributions
- Ion and neutral flux to surfaces

**What range of problems can be tackled with QVT?**

- ✓ Modelling of reactors and tools with complex/novel geometries
- ✓ Investigation of power sources with multiple frequencies and fields
- ✓ Spatial monitoring of simple to complex plasma chemistries
- ✓ Investigation of the surface physics of interesting or novel materials

**The key Advantages of using Q-VT?**

- Wraps the industry standard HPEM code developed by Professor Mark Kushner
- Accessible GUI for full user control over all modules
- Computation times are fast
- **Cost-effective in optimizing processes or implementing new ideas – risk free!**

# Quantemol-N capabilities: Electron - molécule and collision cross-sections

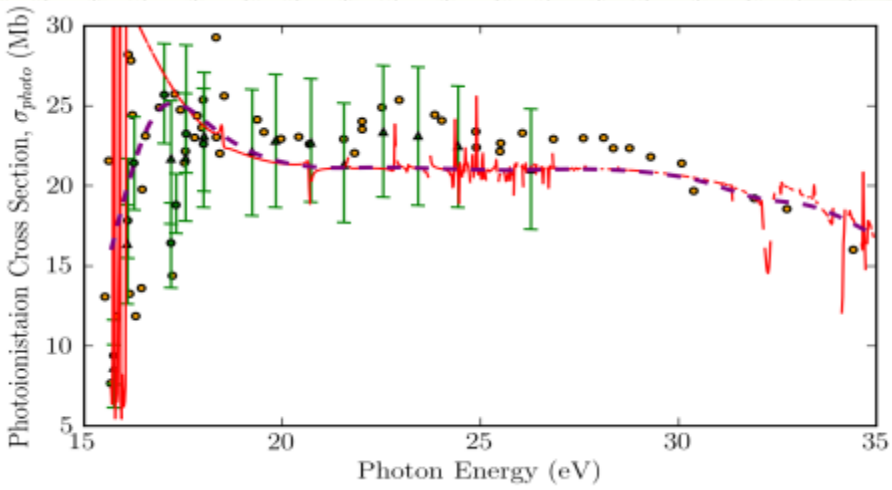
Electron Scattering

**Cross-sections which can be calculated with Q-N 6.1:**

- Elastic scattering
- Electronic excitation
- Super-elastic collisions
- Quenching
- Electron impact dissociation
- Photoionization cross-sections
- Orientated molecule cross-sections
- Rotational excitation
- Electron impact ionization
- Electron attachment
- Momentum transfer
- Differential cross-sections
- Scattering reaction rates
- Resonance parameters

**What range of problems can be tackled?**

- ✓ Closed shell molecules
- ✓ Open shell molecules and radicals
- ✓ Neutral and positively charged species
- ✓ Molecules with up to 17 atoms tested
- ✓ Cross-sections for oriented molecules
- ✓ Calculation of for isotopes



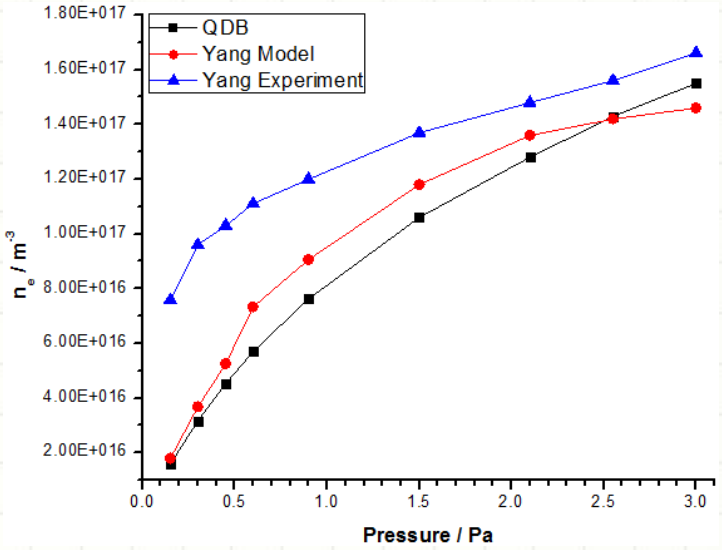
# Quantemol-Database: A repository for plasma chemistries and cross-section data

## QDB Development:

- Similar to NIST, QDB acts as a trusted and centralized source for plasma chemistry information
- Supports and compares multiple datasets
- Developed for those with an interest and/or working on processes that involve complex chemistry
- Developed both for academic research and for industrial research
- Contains cross-section data of electron-atom/molecule collisions
- Data able to be inputted into various modelling software via API

## What does QDB provide?

- ✓ Ongoing data updates and support
- ✓ Self consistent and validated chemistry sets
- ✓ One centralized environment to exchange data and ideas




**$H_2$ Plasma discharge validation**

# Conclusions

- Modelling is great!!! ☺
- Modelling helps reduce costs whilst increasing the workspace for innovation
- Fundamental understanding and the fleshing out of ideas are encouraged via the use of 0D, 2D and 3D modelling codes for plasma chemistry and reactor tool development
- Data from modelling can be easily shared and used without having to dedicated time and resources to making prototypes that may or may not work
- In a climate where the industry is very competitive, modelling is a necessary step to ensure companies stay ahead of the game.