

# Atomic Physics in ITER

The Foundation for the  
Next Step to Fusion Power

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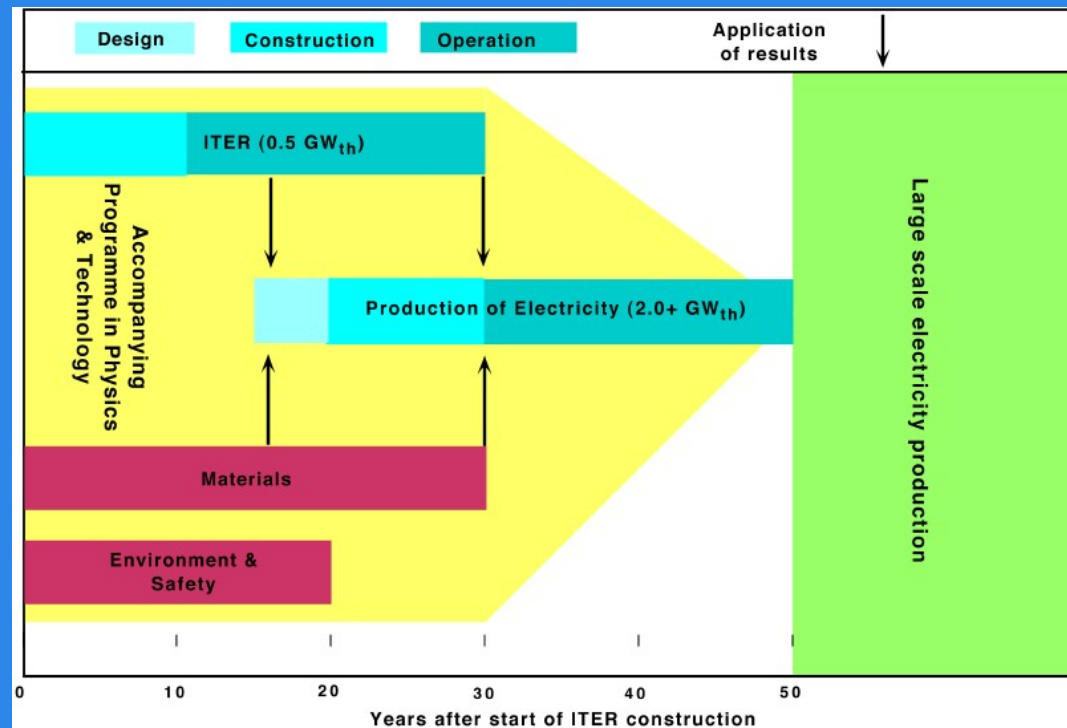
The 5<sup>th</sup> International Conference on Atomic  
and Molecular Data and Their Applications  
Meudon, France, October 15-19, 2006

# ITER



# ITER Will Demonstrate Scientific & Technological Feasibility of Fusion Power

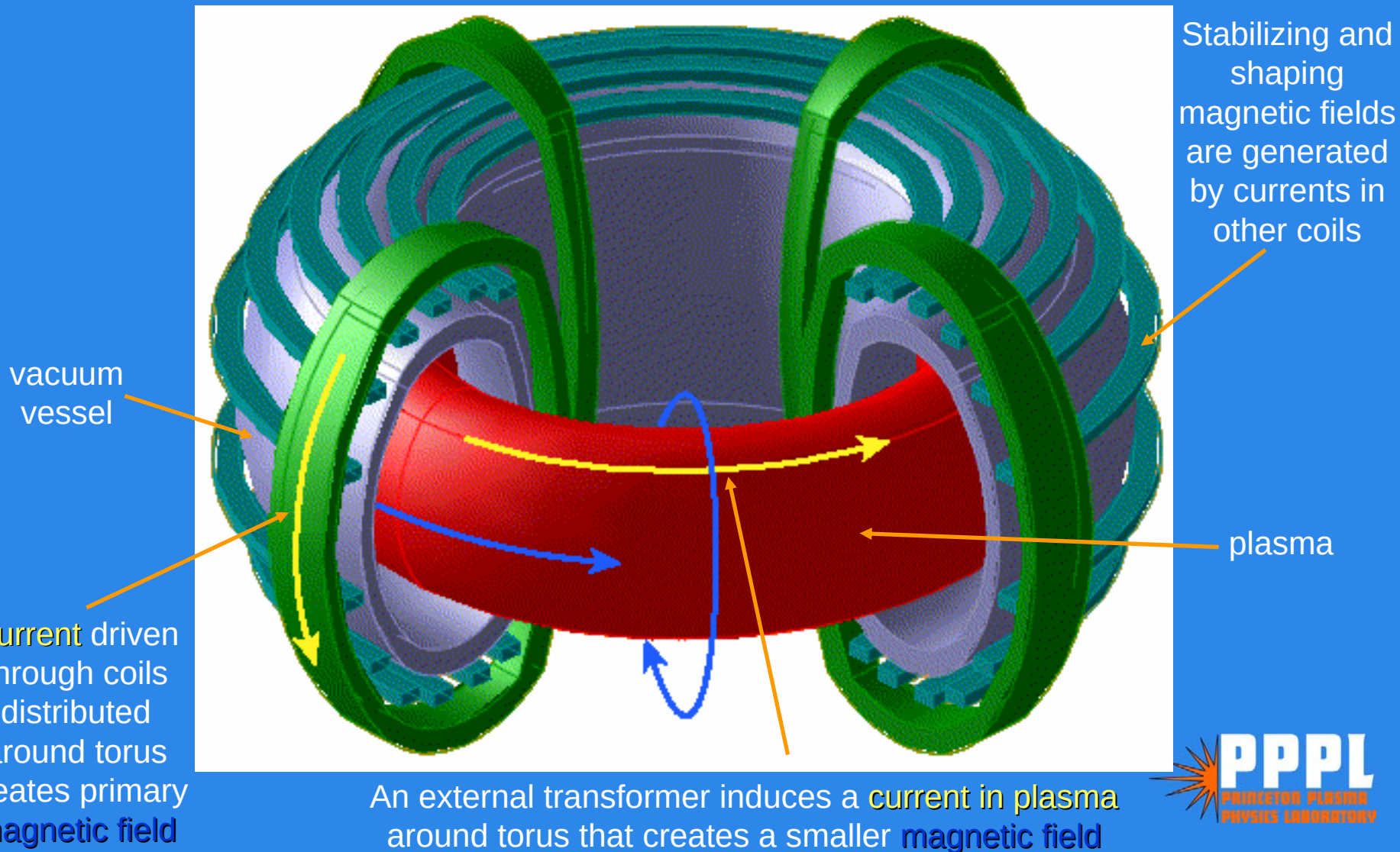
- Produce & control burning fusion plasma for extended periods of time [ITB 2002, IPB 1999].
- Test reactor relevant technologies:
  - Superconducting magnets,
  - High heat & neutron flux components,
  - Remote maintenance.
- ITER will not generate net electricity,
  - But, will test power reactor blanket modules,
  - And tritium breeding concepts.
  - ITER will also need to “recycle” tritium on site.



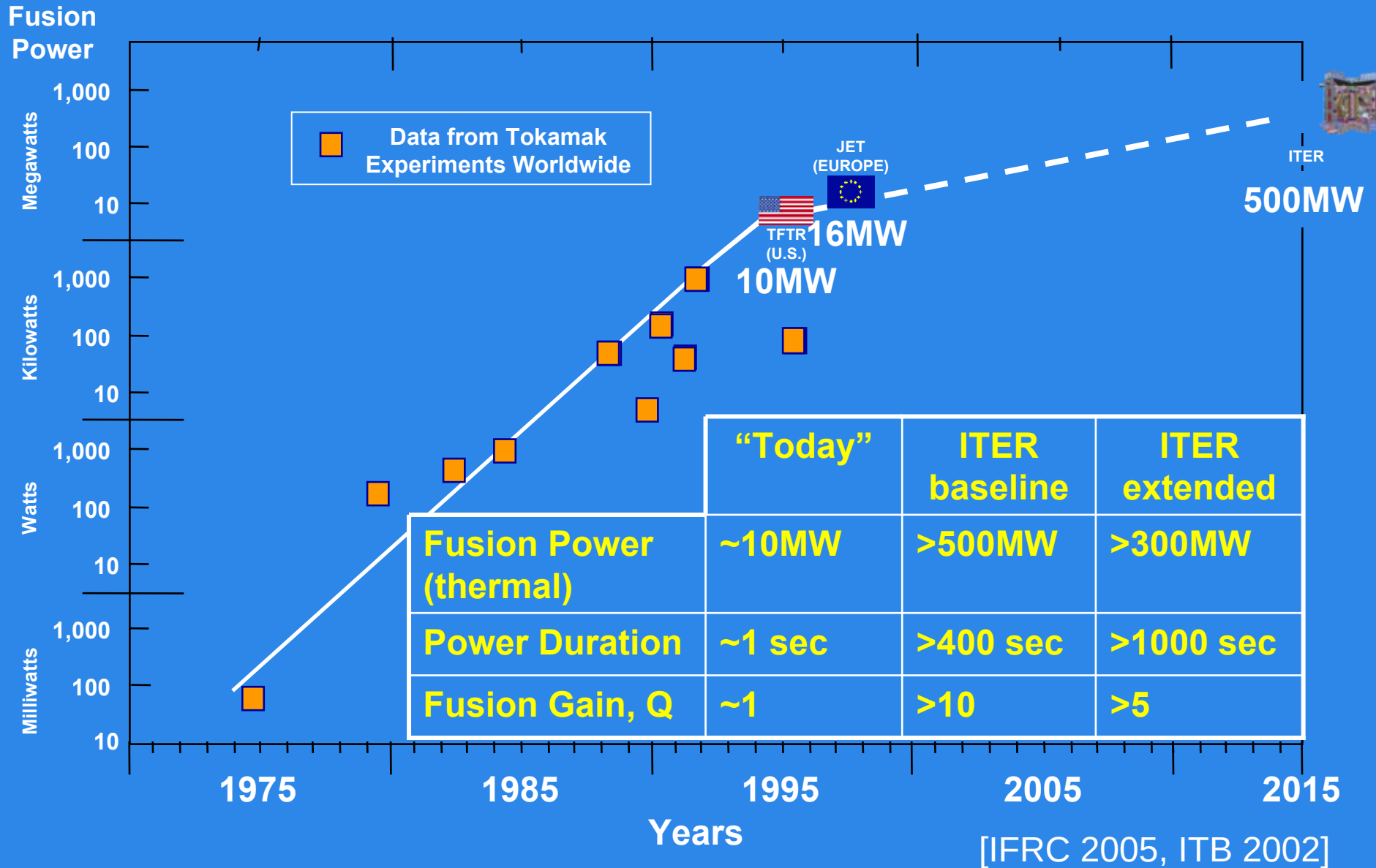
[Smith 2004, IFRC 2005, Socolow 2006]



# The Most Successful Magnetic Confinement Configuration is the Tokamak



# ITER's Fusion Performance in Context



**ITER:  $R = 6.2$  m,  $a = 2.0$  m,  $V_p = 850$  m<sup>3</sup>**  
 **$I_p = 15$  MA,  $B_T = 5.3$  T,  $W_{\text{mag}} = 41$  GJ**

Central  
Solenoid,  
Nb<sub>3</sub>Sn

Toroidal  
Field Coil,  
Nb<sub>3</sub>Sn

Poloidal  
Field Coil,  
NbTi

Gravity  
Support

Standard  
Man

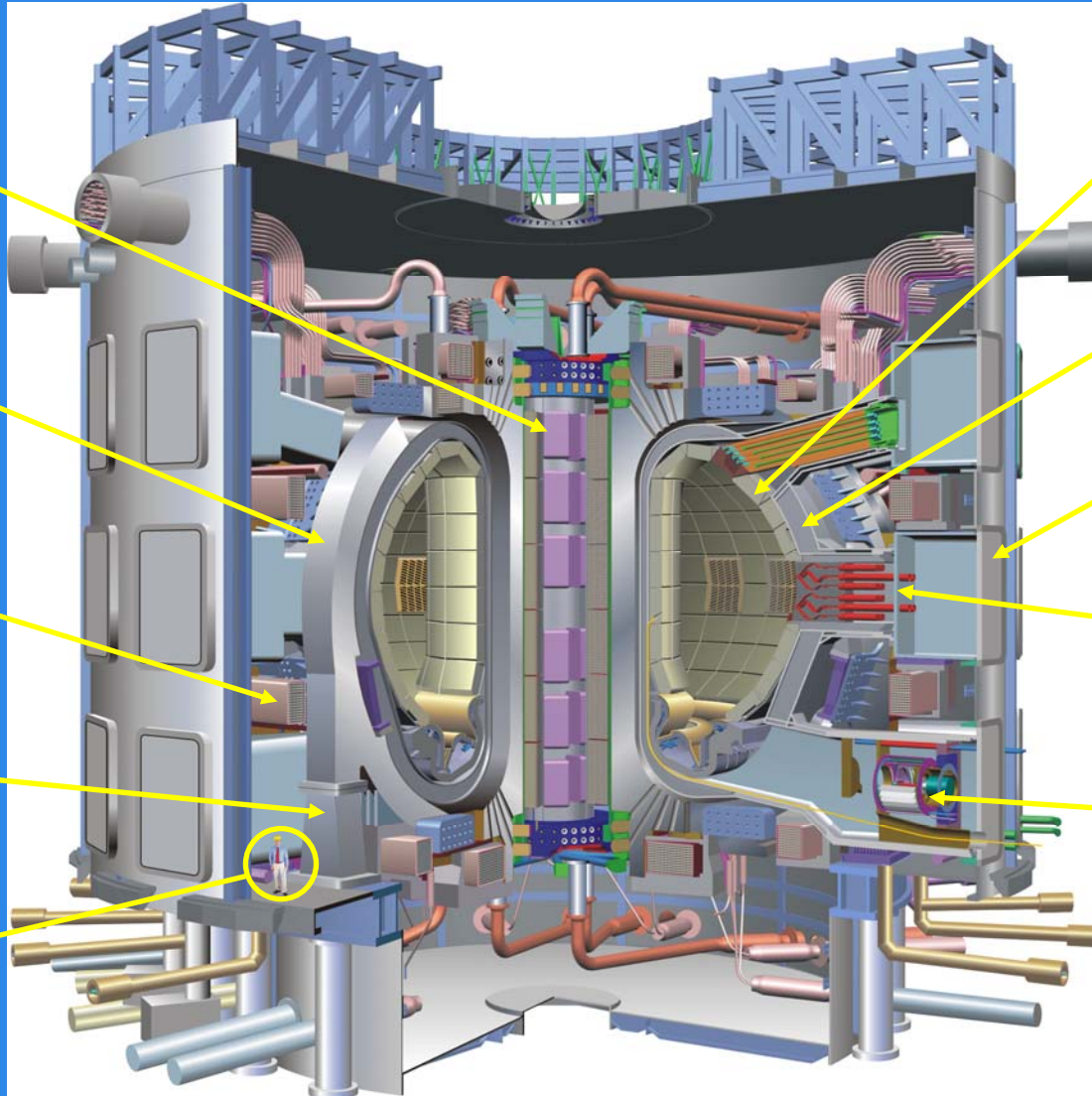
Blanket  
Module

Vacuum  
Vessel

Cryostat

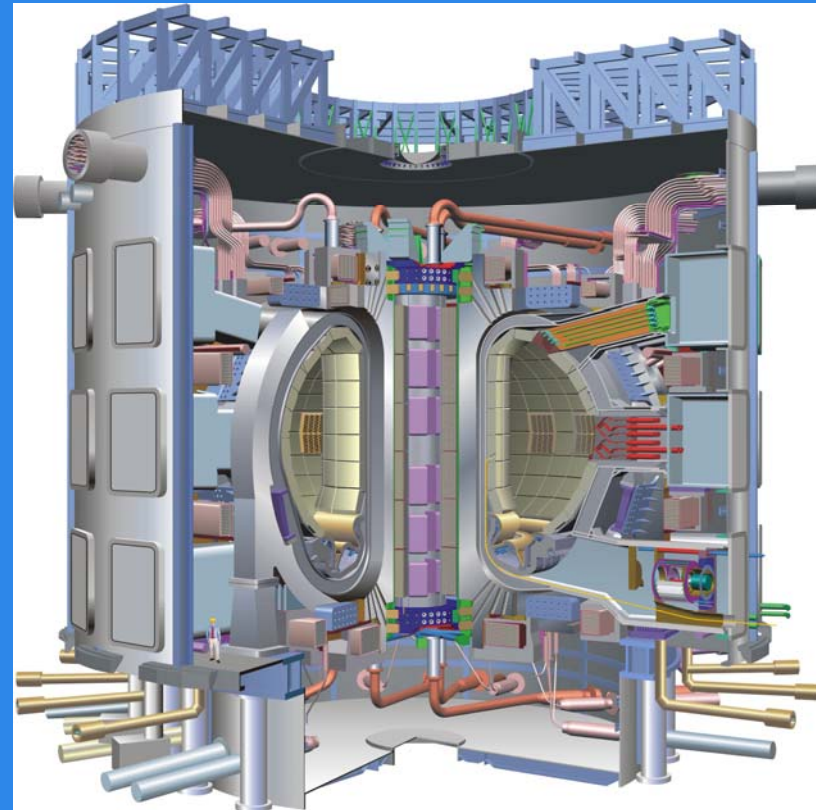
Port Plug  
(IC Heating)

Torus  
Cryopump

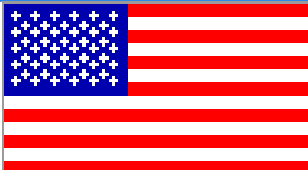
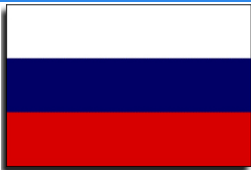
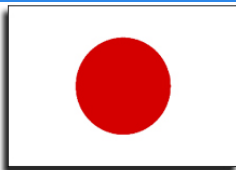


# In May 2006, the ITER International Agreement was Initialed

- **The partner governments:**
  - Have judged sufficient scientific and technological readiness and benefits,
  - Are committing 110% of the ITER value for construction,
  - Have agreed on the hardware responsibilities of each party,
  - Have developed organizational and legal arrangements for the ITER Legal Entity.
- **International agreement was initialed in May; signing is planned for November 21.**
- **Transitional activities are underway.**



<http://www.iter.org>





# Outline

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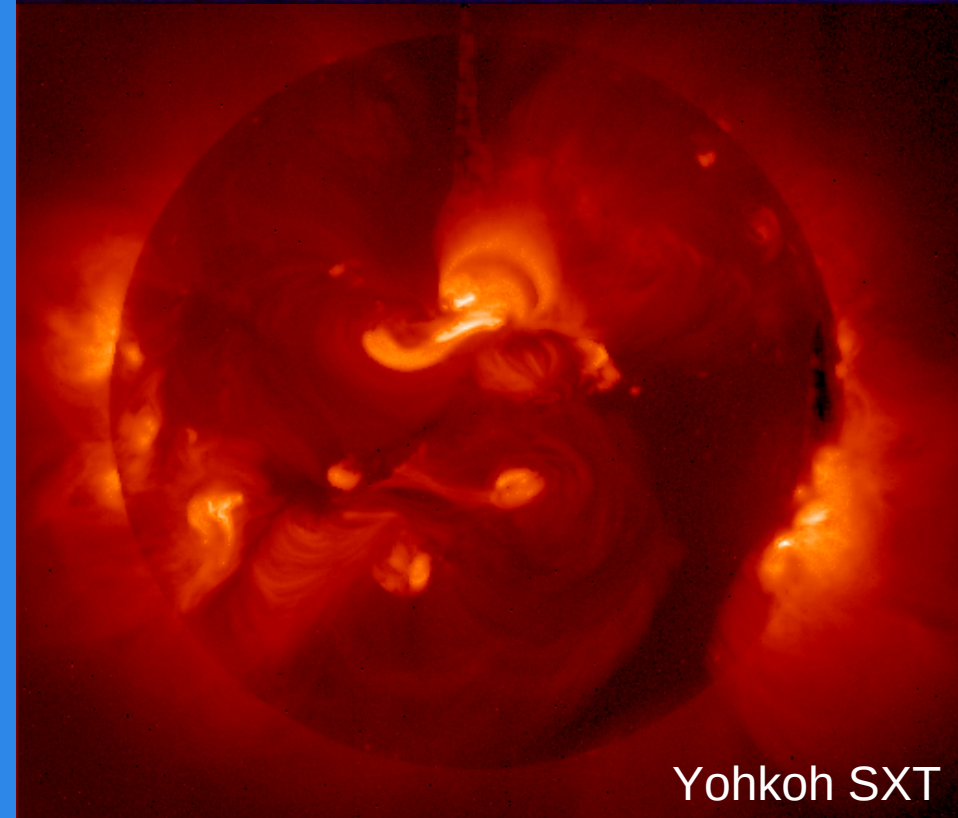
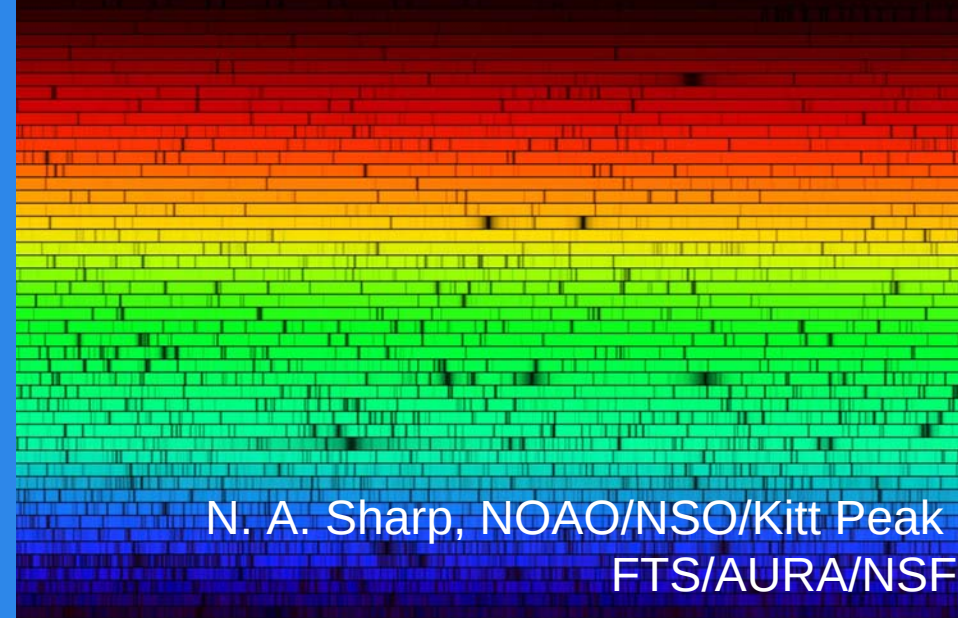
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- 2. Boundary of Tokamak Plasmas**
- 3. Atomic Physics in the Edge & Divertor Plasmas**
  - A. Recycling**
  - B. Radiating Mantle**
- 4. Atomic Physics in Core Diagnostics**
  - A. CX Recombination Spectroscopy**
  - B. Motional Stark Effect**
  - C. X-ray Crystal Spectroscopy**



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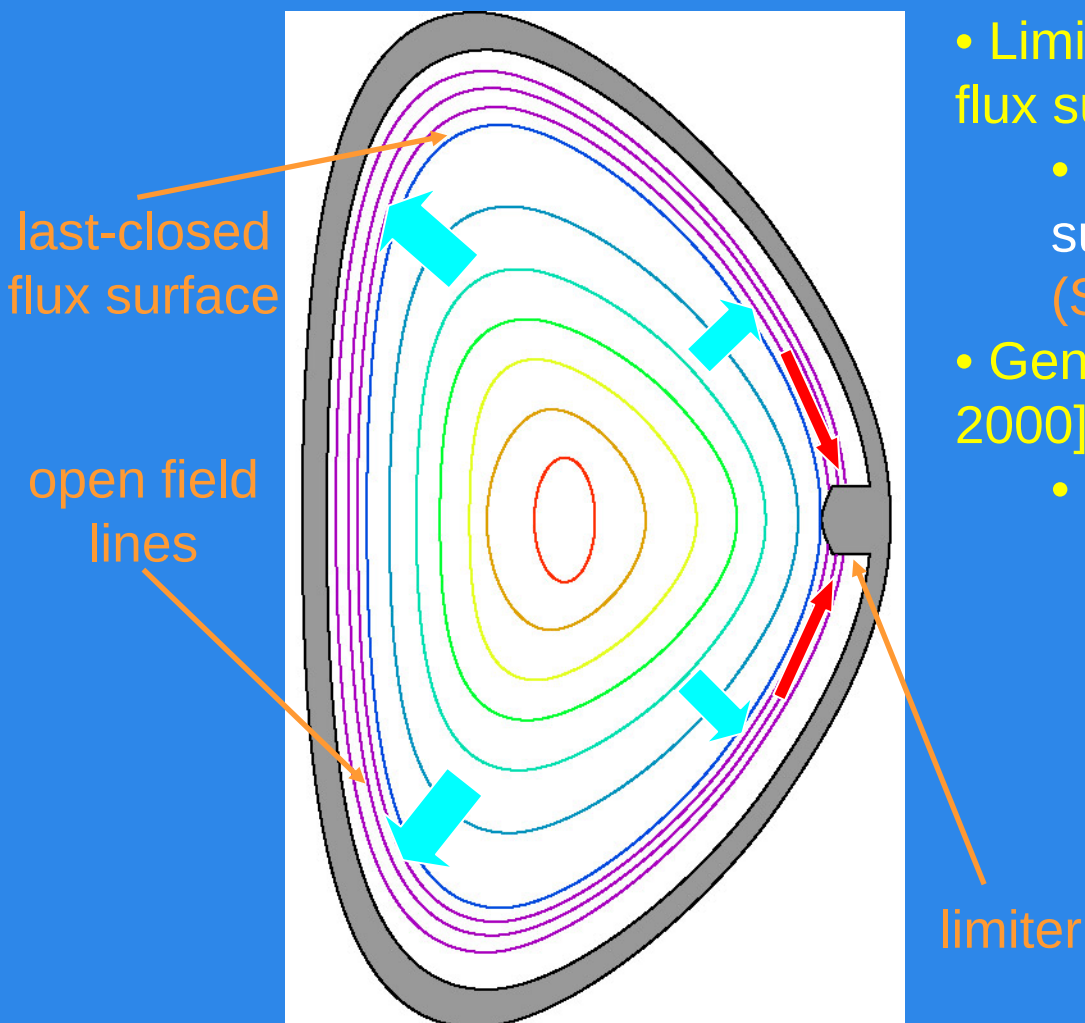


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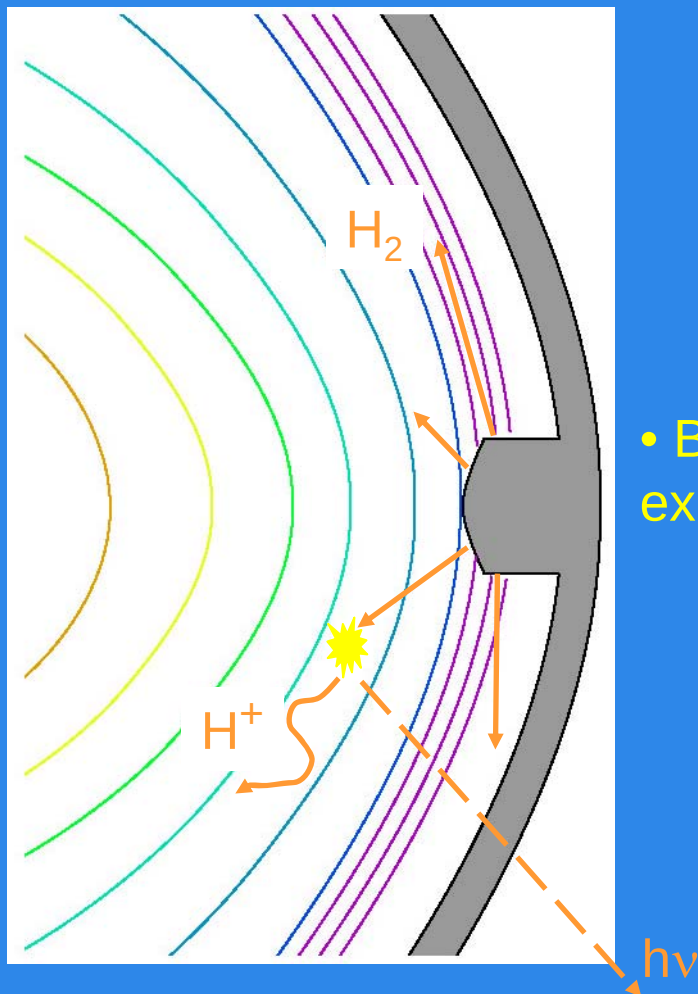


# Simplest Plasma-Material Interaction Configuration Is the Limiter



- Limiter location defines last-closed flux surface,
  - Intercepts open field lines / flux surfaces  $\Rightarrow$  scrape-off layer (SOL).
- General reference: [Stangeby 2000],
  - See also: [Reiter 2005].

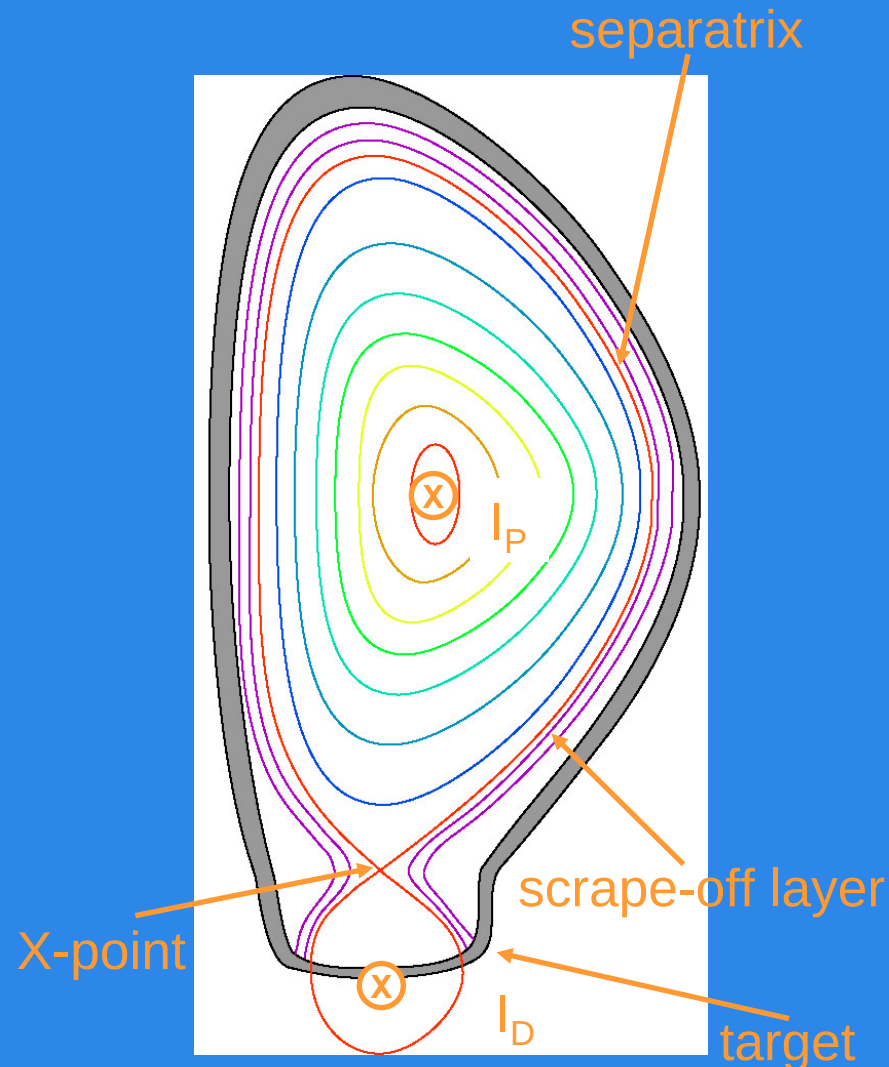
# Limiter Acts as a Sink for Plasma Particles and Power



- Not for mass, however:
  - Electrons & ions recombine at surface,
  - In steady-state, resulting neutral atoms & molecules recycle back into plasma.
  - Neutrals travel freely across field lines,
  - & be ionized near or far from limiter
  - $\Rightarrow$  plasma can refuel itself.
- Before being ionized, H atoms can be excited by electron impact,
  - Radiatively decay & emit photons,
  - $\Rightarrow$  Markers of ionization.
  - E.g.,  $n = 3 \rightarrow 2$  transition (Balmer-alpha or  $H_\alpha$ ) at  $\sim 6560 \text{ \AA}$  dominates visible emissions & is often used for diagnostics.

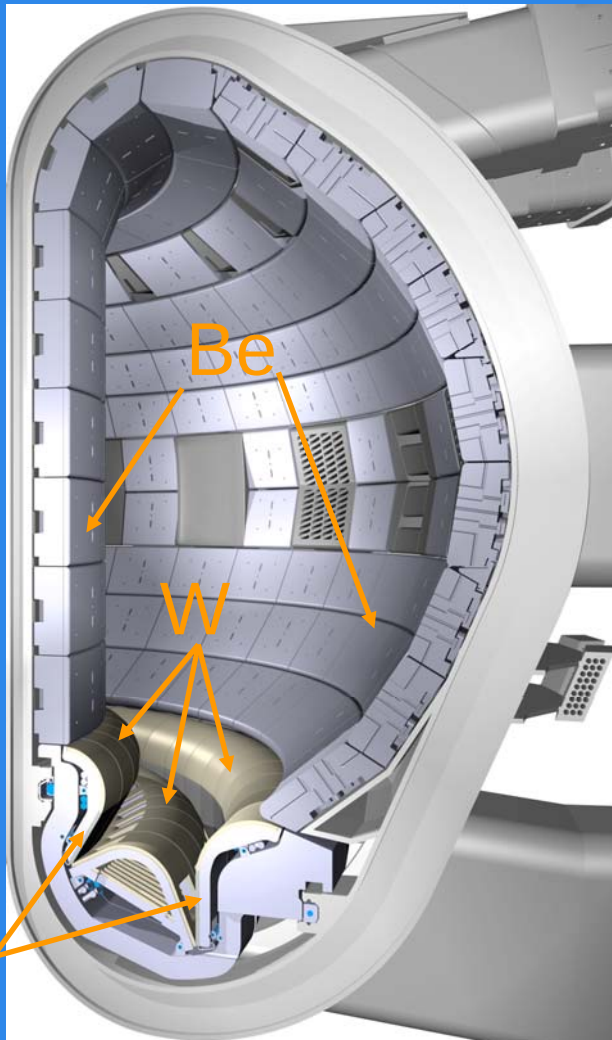


# Tokamak Divertor Configuration Moves the Plasma Material Interaction Away From Core



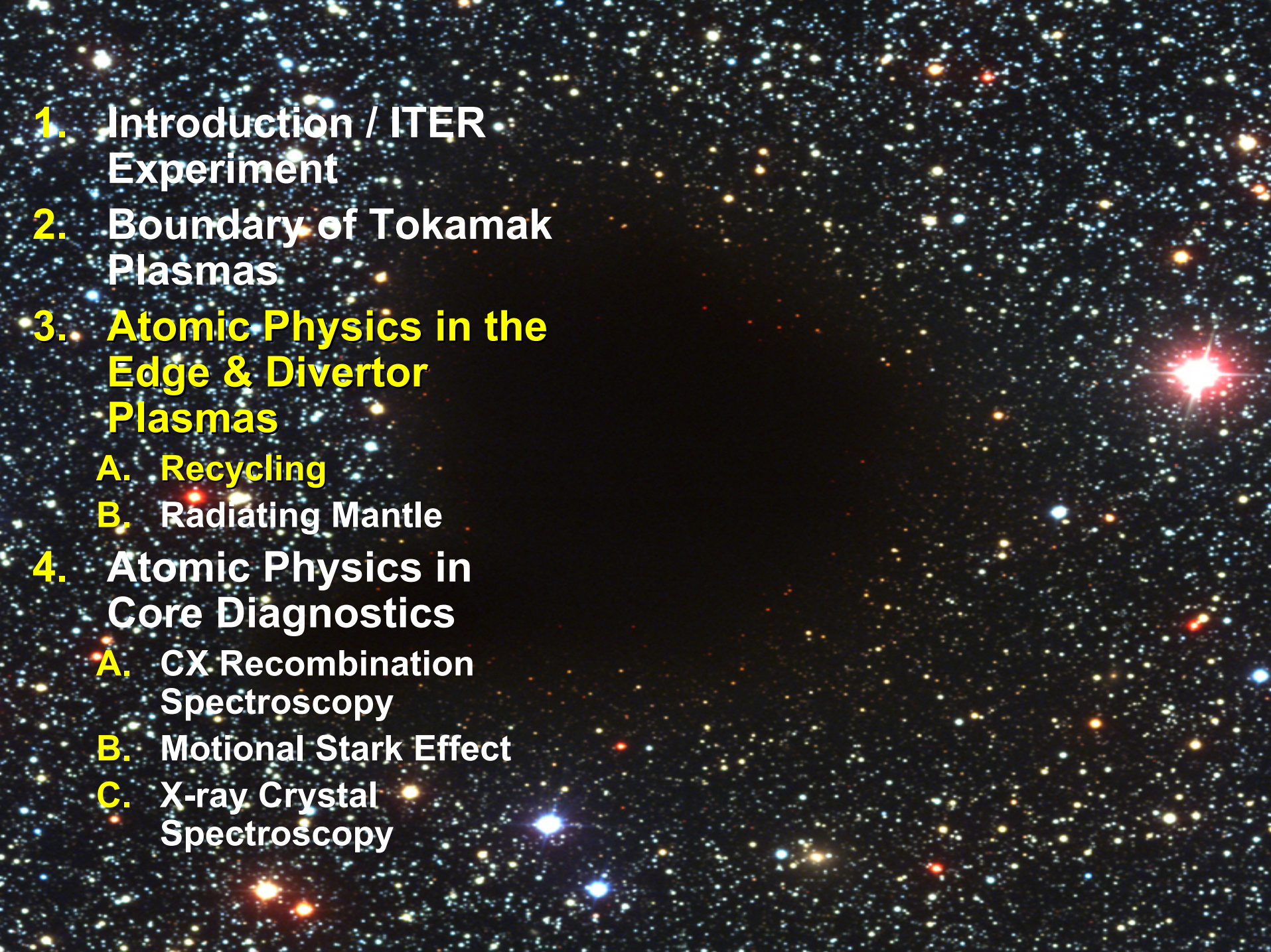
- Divertor created by adding coil  $I_D$  with current in same direction as  $I_P$ .
- In between, get  $B_{pol}=0$ .
  - This is the **X-point**.
  - Corresponding surface is **separatrix**; becomes the LCFS.
  - Separates **SOL** from **core** plasma.
- SOL field lines strike material surface at the **divertor targets**.
- Divertors concentrate particles & power.
- Facilitates pumping,
- But complicates power handling!

# ITER Will Use a Mix of Plasma Facing Materials



- **Main chamber: Be.**
- **Divertor surfaces mostly W,**
  - Except for target strike points, C.
- **Existing tokamak database dominated by all carbon machines,**
  - More aggressive research with ITER relevant materials under way.
- **Divertor plasma parameters:**
  - $n_e = 10^{20} - 10^{21} \text{ m}^{-3}$ ,
  - $T_e = 0.1 - 100 \text{ eV}$ ,
  - $n_D = 10^{19} - 10^{20} \text{ m}^{-3}$ ,
  - $P_{D2} = 0.1 - 10 \text{ Pa (plenum)}$ .



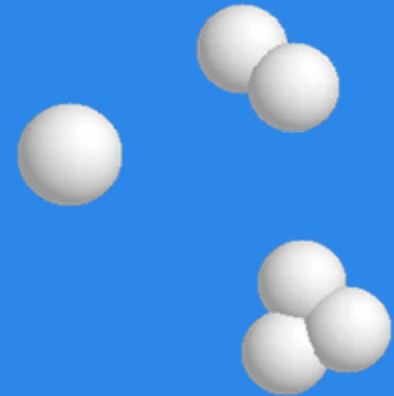
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# Atomic Physics Processes Mediate Exchange of Mass, Momentum, & Energy Between Plasma & Neutrals

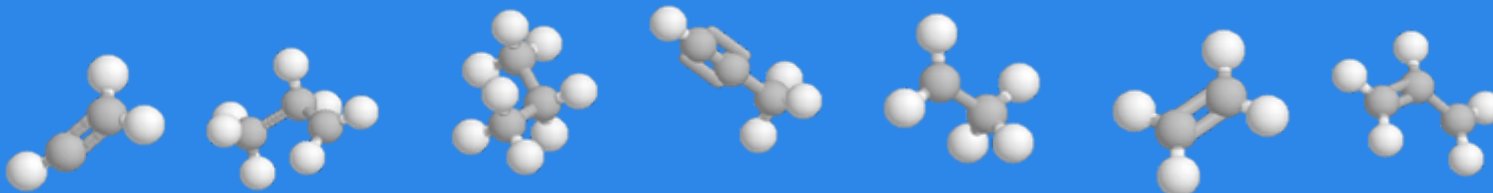
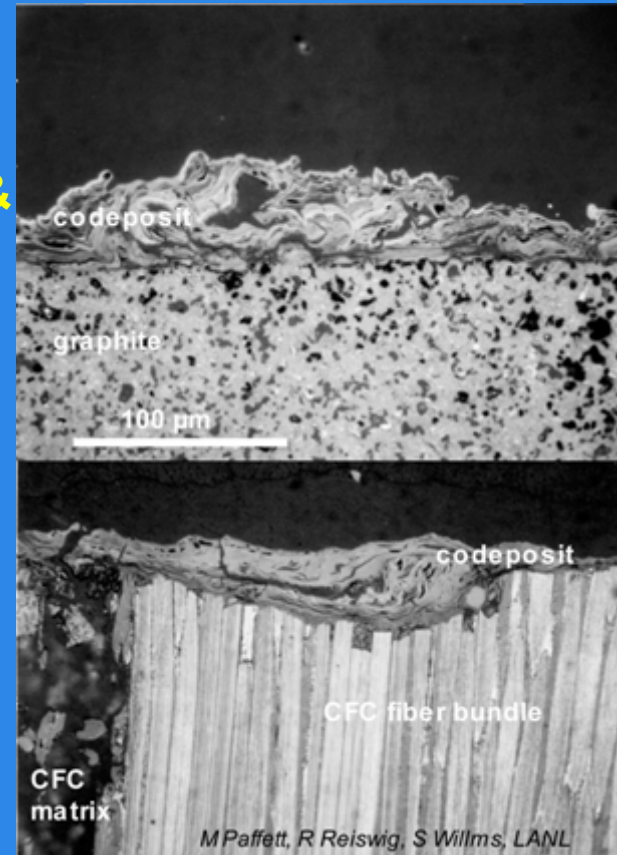
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- **H CR ionization & recombination,**
  - H & H<sup>+</sup> not in equilibrium! [Reiter 1993]
- **Elastic scattering of H, H<sub>2</sub> on H<sup>+</sup>,**
  - Fully quantal dσ/dΩ [Krstic 1998, Stotler 2001],
  - Momentum transfer to H<sub>2</sub> crucial.
- **H<sub>2</sub>, H<sub>2</sub><sup>+</sup> dissociation, ionization,**
  - Basic processes: [Janev 1987].
- **Vibrational excitation ⇒ ion conversion, H<sub>3</sub><sup>+</sup>, H<sub>3</sub><sup>-</sup>, ...**
  - Became relevant with higher n<sub>e</sub>, lower T<sub>e</sub> divertors,
  - Need combined atomic & molecular CR model [Fantz 2001].
  - Assessment: more data needed [Janev 2003].
- **Neutral – neutral collisions (viscosity),**
  - Significant in highest density experiments (& ITER [Kukushkin 2005]).
- **Lyman-α radiation trapping by H,**
  - Need self-consistent simulation of plasma, gas, and radiation [Reiter 2002],
  - With detailed line profiles [Adams 2004].
- **For an example: see [Reiter 2005].**



# Will Need to Understand Hydrocarbon Behavior

- **Safety concerns limit amount of in-vessel tritium in ITER [Federici 2001],**
  - Trapped in redeposited hydrocarbons,
  - Extrapolation of existing data  $\Rightarrow$  serious problem.
- **Mechanisms of hydrocarbon creation, transport, & deposition not completely understood.**
- **Starting point: data for dissociation & ionization of hydrocarbons improving,**
  - $\text{CH}_y$ ,  $\text{C}_2\text{H}_y$ ,  $\text{C}_3\text{H}_y$  [Janev 2002, Janev 2004],
  - See also HYDKIN reaction analysis tool:  
<http://www.eirene.de/eigen/index.html>
- **Resulting system very complicated!**
  - ~500 processes!
  - Need to reduce to a simpler model for use in simulations.
  - May not be possible in general [Reiter 2006].
- **Tritium removal techniques also being pursued.**



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# Can Estimate Heat Flux Striking Material Surfaces in ITER

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- **ITER objective:  $Q = 5 \rightarrow 10$ ,**
  - $Q = 10, P_{\text{fus}} = 500 \text{ MW} \Rightarrow P_{\alpha} = 100 \text{ MW}, P_{\text{in}} = 50 \text{ MW}, P_{\alpha} + P_{\text{in}} = 150 \text{ MW}.$
- **How to exhaust 150 MW from plasma to surrounding materials?**
  - Plasma will carry it along field lines,
  - Area of divertor target receiving plasma flux determined by plasma through competition between parallel (classical) and perpendicular (turbulent) transport,
    - Latter not well understood  $\Rightarrow$  just have models for ITER.
  - Extrapolate empirical models:  $\geq 2 \text{ m}^2$  [Herrmann 2003],
  - $\Rightarrow 75 \text{ MW/m}^2$  heat flux.

# Use Impurity Atoms to Radiate Power Over Larger Area

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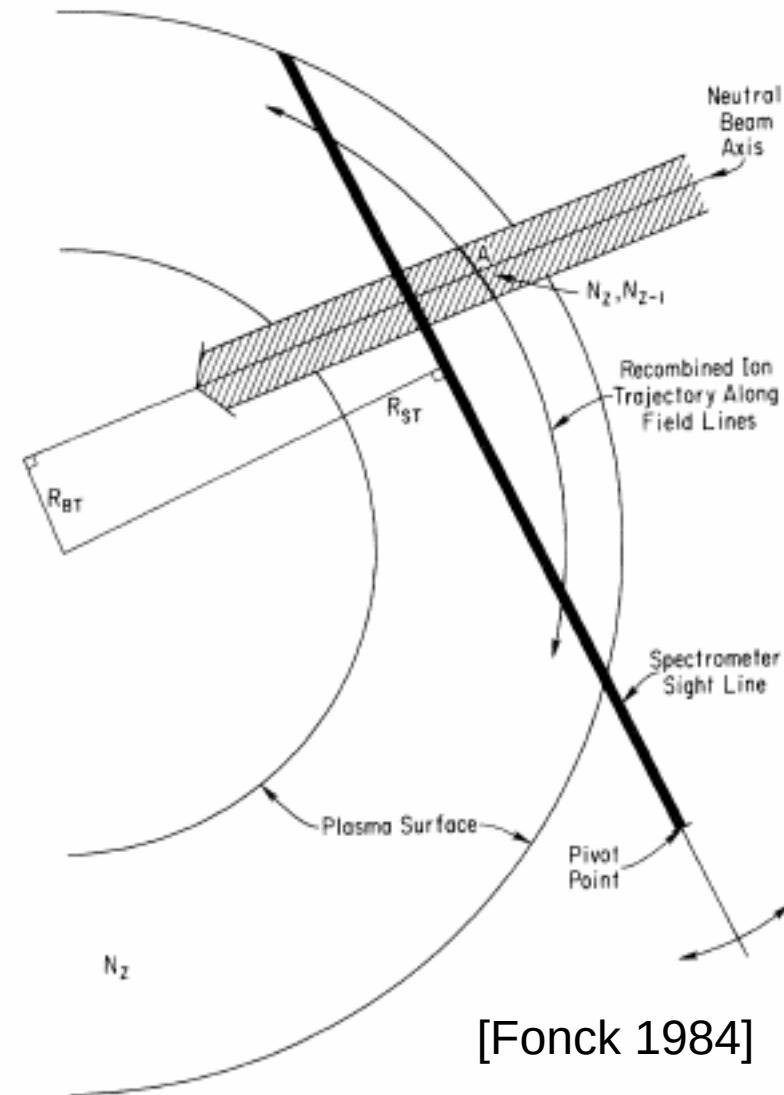
- Would like to radiate ~75% of the power [Kukushkin 2005].
- Where radiation takes place matters:
  - Too far into core  $\Rightarrow$  occurs at expense of fusion reactions,
  - Too close to divertor targets  $\Rightarrow$  power still concentrated,
  - Ideal: radiating mantle just inside last closed flux surface,
  - Even there, too much radiation spoils core confinement.
  - Modeling shows radiation in edge, SOL, and divertor reducing heat load to 10 MW/m<sup>2</sup> [Kukushkin 2002].
- “Recycling” extrinsic impurities prevent in-vessel accumulation of deposits in steady-state,
  - E.g., noble gases: Ne, Ar, Kr, Xe; also N<sub>2</sub>.
  - Using gases makes controlled introduction easier.
- Atomic physics data used for modeling impurity radiation appear in good shape,
  - But, in most present day devices, C is dominant impurity.

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# Charge Exchange Recombination Spectroscopy $\Rightarrow n_i, T_i, v_i$

- Spectroscopy of optical transitions from CX of injected neutral beam with fully stripped impurity ions in core [Isler 1994],
  - $H + A^{+q} \rightarrow H^+ + [A^{+(q-1)}]^*$
- Use fully stripped ions:
  - That's what's in the core!
  - Resulting ion is H-like.
- Beam energy must be high enough to penetrate to core,
  - Use heating beam
  - Or dedicated diagnostic beam.
- Ideally, use data for CX into  $(n,l)$  states of  $A^{+(q-1)}$ ,
  - Cross sections primarily calculated.
  - But, plasma can mix nearly degenerate states.
  - Also need rates for cascade towards ground state & corresponding emission.



[Fonck 1984]

# Interpreting Resulting Spectrum Requires Accounting for Many Complicating Effects

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- **Contributions by “halo” H atoms [Isler 1994],**
  - Thermal  $H^+$  that has CX'd with beam,
  - Can in turn CX with impurity ions.
- **“Plume” ions are  $[A^{(q-1)}]$  ions created by CX on another flux surface [Fonck 1984],**
  - Can drift into sight line and be excited by electrons,
  - $\Rightarrow$  Contribute at different temperature.
- **Beams have significant  $1/2$  &  $1/3$  energy components from  $H_2^+$  &  $H_3^+$  in source,**
  - **Need CX cross sections at lower energies to take these into account.**
- **Beam atoms can be in excited states [Isler 1994],**
  - Small fractions, but much larger cross sections!
- **Gyro-orbit dependence [Bell 2000],**
  - Combine with  $\sigma(E)$  & finite lifetimes to complicate velocity measurements,
  - $\Rightarrow$  Need kinetic treatment of ions rather than fluid.
  - Multiple views help sort out these effects.

# CXRS Issues for ITER

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- **ITER active beam spectroscopy:** [Malaquias 2004, von Hellermann 2004].
- **Should have multiple views to sort out gyro-orbit effects.**
- **Need (n,l) resolved cross sections,**
  - And at energies low enough to account for  $\frac{1}{2}$  &  $\frac{1}{3}$  beam energy contributions.
  - Heating beam: 500 keV/amu, DNB: 100 keV/amu.
- **Take plume emission into account for He measurements,**
  - Essential to track flow of ash.
- **C & Be coatings will degrade first mirrors over time,**
  - $\Rightarrow$  Will need some method of tracking reflectivity & polarization over time.
  - Or in situ cleaning.



# Motional Stark Effect → Spatially Resolved Measurements of Magnetic Field Orientation

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- **Tokamak magnetic field consists of poloidal & toroidal components,**
  - Poloidal field due to plasma currents ⇒ determined self-consistently within plasma & cannot be computed a priori.
  - ⇒ Important measurement to aid in equilibrium reconstruction and in testing theories of plasma equilibrium, stability, and transport.
- **MSE diagnostic also relies on heating or diagnostic beam,**
  - Consider Balmer- $\alpha$  emissions due to excitation of beam atoms by background plasma.
  - Stark effect associated with  $E = V_{\text{beam}} \times B$ ,
  - ⇒ wavelength splitting of several angstroms & polarization of emitted radiation [Levinton 1989].
- **Initial applications on PBX-M & TFTR measured direction of polarization ⇒ local  $B_p/B_T$  [Levinton 1993].**
- **As with CXRS, single beam with multiple sight lines ⇒ profile of  $B_p/B_T(r)$ .**

# MSE Issues for ITER

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- **Mirror coatings may prevent accurate polarimetry  
⇒ considering alternatives.**
  - Namely, precision spectrometry.
  - Line shifts much less sensitive to changes in reflectivity,
  - Investigating prospects for getting enough data from them to measure field line pitch.
- **Developing CR model including (n,l) sublevels,**
  - **Need correspondingly detailed cross sections,**
  - Do these exist?
- **Another approach based on measurement of ratio of  $\pi$  and  $\sigma$  line components has been proposed [von Hellermann 2004, Malaquias 2004],**
  - Will require isotropic reflection throughout optical system.

# Independent Measurements of Plasma Parameters Always Desired!

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- **E.g., X-ray spectroscopy can also give  $T_i$  and flow velocity,**
  - Looks at emission lines from higher Z impurities than CXRS: Kr, Ar, W, etc.
  - Considering He-like & H-like Kr, Ar, Fe for ITER [Barnsley 2004],
    - Spectra for these are in good shape.
    - Amount added limited by increment in  $P_{\text{rad}}$ .
    - Free-free & free-bound continuum emission is important source of noise in ITER!
- **W may be more problematic,**
  - Used for divertor target plates  $\Rightarrow$  intrinsic impurity.
  - Need reliable energy levels, emission rates,...
  - Models can be tested on existing experiments: ASDEX-U (now), JET (coming soon).



# Summary

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- **ITER is an ambitious project,**
- **In the process of designing & preparing to build it, we're testing existing models and developing new ones more aggressively than ever before.**
- **This is especially true for the edge & divertor plasmas,**
  - It's here that our knowledge of atomic physics is crucial to the project's success,
  - In dealing with plasma-wall interactions, taming problems like tritium retention, and spreading out exhaust power.
- **Much work also remains to be done on the atomic physics aspects of ITER's core diagnostics,**
  - We will need to be confident in interpreting their signals to gauge ITER's performance.

**Acknowledgements: this talk improved immensely by conversations with Detlev Reiter, Ralf Schneider, Dave Johnson, Ron Bell, Fred Levinton, and Ken Hill.**

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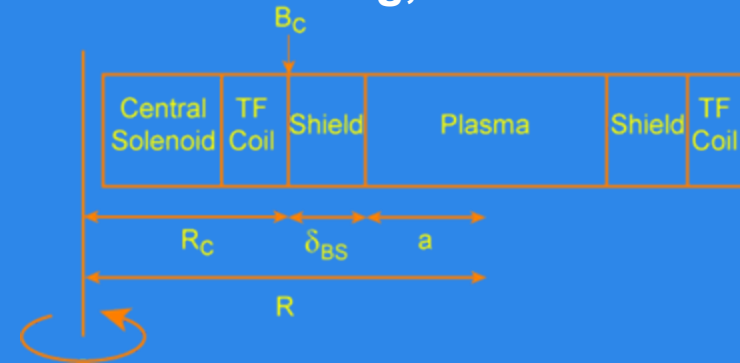
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- [Stotler 2001] D. P. Stotler et al., "Modeling of Alcator C-Mod Divertor Baffling Experiments", *J. Nucl. Mater.* **290-293**, 967 (2001).
- [von Hellermann 2004] M. von Hellermann et al., "Pilot Experiments for the International Thermonuclear Experimental Reactor Active Beam Spectroscopy Diagnostic", *Rev. Sci. Instrum.* **75**, 3458 (2004).

# **Supplementary Slides**

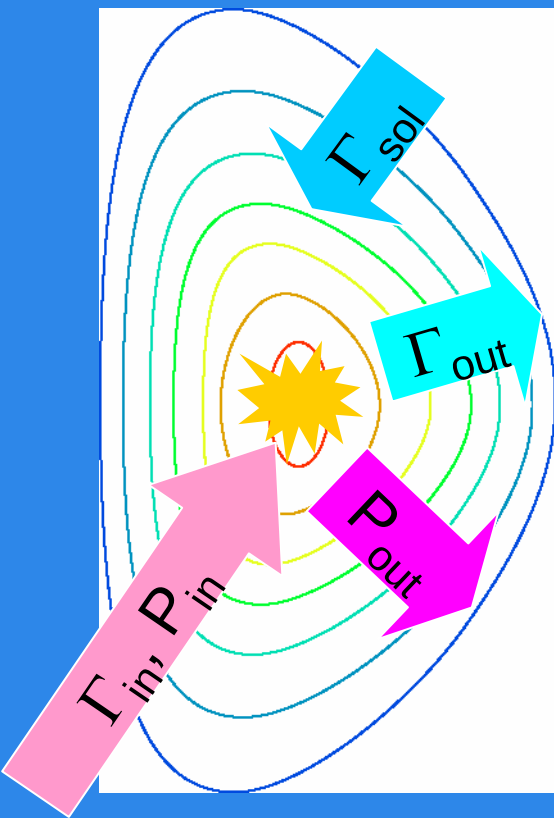
# What Is Holding Up Fusion Progress?

- **Alternatively: Why is ITER So Big?**
- **Years of tokamak confinement experience + fusion cross section**  $\Rightarrow P_\alpha / (P_\alpha + P_{in}) \propto [I_p (R/a) H / 46]^3$ ,
  - H: multiplier on empirical energy confinement time scaling,
  - Assumes  $T_i \cong 10$  keV.
- **Tokamak radial build**  $\Rightarrow R = R_c + \delta_{BS} + a$ ,
  - $R_c$  = radius at TF coil,
  - $\delta_{BS}$  = Blanket / shield thickness = 1.3 m.
- **Ampere's Law**  $\Rightarrow R = R_c B_c / B_T$ ,
  - $B_c = 12$  T for  $Nb_3Sn$ .
- **Macroscopic stability**  $\Rightarrow$  Safety factor  $q = 5 a^2 B_T f / R I_p \cong 3$ ,
  - Shape factor  $f \cong 2.3$ .
- **Conventional tokamak**  $\Rightarrow R / a = 3$ ,
  - With  $I_p (R/a) = 46 \Rightarrow a = 2.0$  m,  $R = 6.4$  m,
    - But, no margin for fuel dilution, less than expected confinement, ...
  - ITER EDA:  $I_p (R/a) = 60 \Rightarrow a = 2.6$  m,  $R = 7.8$  m.



# In Steady State, Have Power & Particle Flows To Material Boundaries

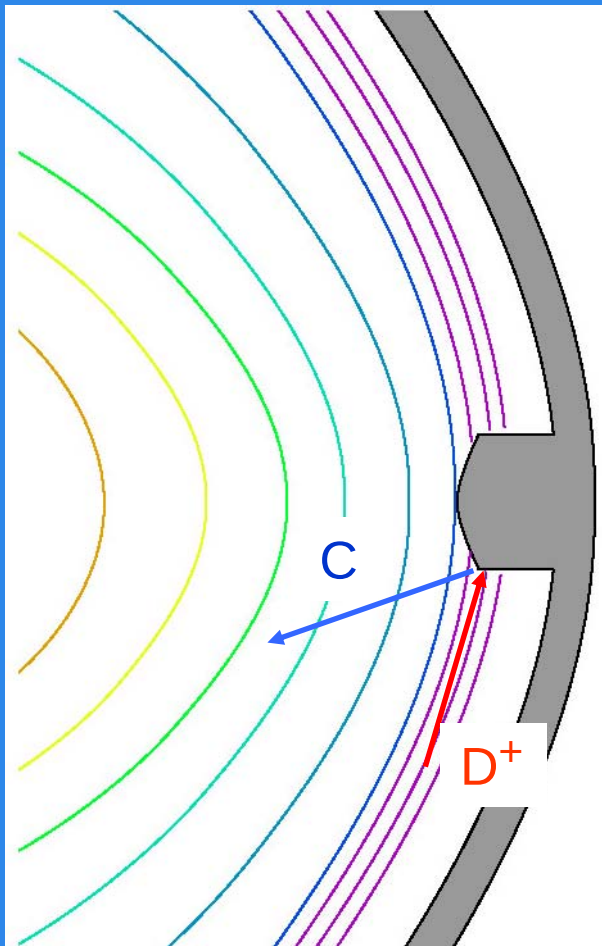
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- In a reactor, 80% of fusion power leaves as neutrons,
  - Captured in blanket.
- Other 20% flows out of plasma & strikes material boundaries.
- Particle flows replace fuel ions & remove He ash.
- In non-DT experiment,  $P_{out} = P_{in}$ ,
- Particle flows determined by competition between sources (core & edge) and diffusion.
- General reference: [Stangeby 2000]



# High $T_e$ Near a Material Can Lead to Impurity Sputtering



- Particles striking a material at high enough energy can knock off substrate atoms  $\Rightarrow$  physical sputtering.
- Becomes a significant particle source for  $E \sim \text{few } 100 \text{ eV} - 1 \text{ keV}$ ,
  - $\Rightarrow$  Is a concern for  $T_e > 100 \text{ eV}$ .
- Can lead to self-sputtering,
  - Efficient due to similar projectile & substrate mass,
  - And due to  $Z > 1$ .
- Sputtered impurities can harm core,
  - Efficient radiators  $\Rightarrow P_{\text{rad}}$ ,
  - Dilute hydrogen fuel.

# Fundamental Set of Atomic Physics Processes & Rates Essentially Unchanged for ~20 Years

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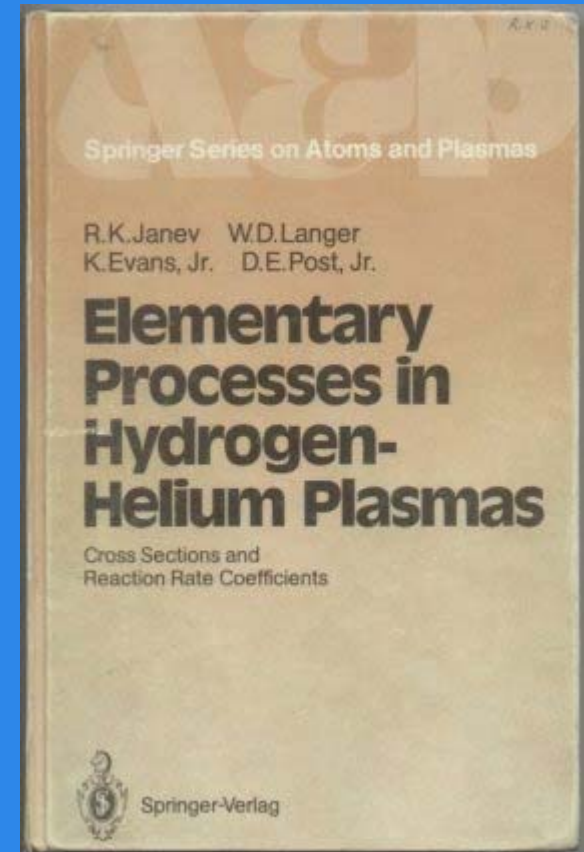
## 1. Dissociation, ionization, etc. of $H_2$ , $H_2^+$

- From [Janev 1987]
- Maxwellian averaged reaction rates as function of  $T_e$ ,
- Simple dissociation energies & energy losses.

## 2. Collisional radiative model for electron impact ionization and recombination of H,

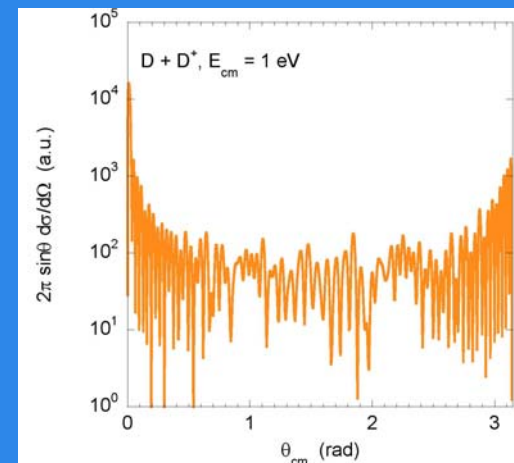
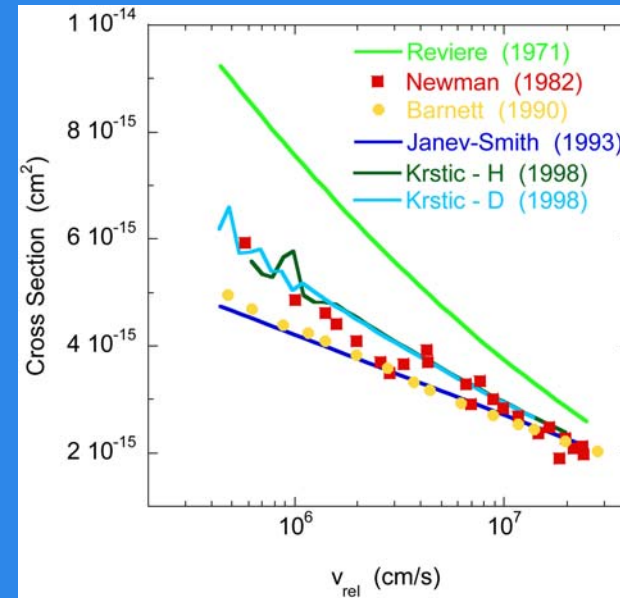
- But, H &  $H^+$  not in equilibrium!
- See [Reiter 1993] & references therein.

$$\frac{Dn_0}{Dt} = -n_0n_eS_{\text{eff}} + n_in_eR_{\text{eff}}$$



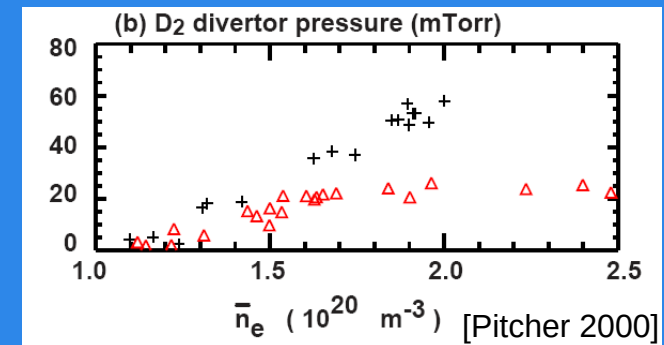
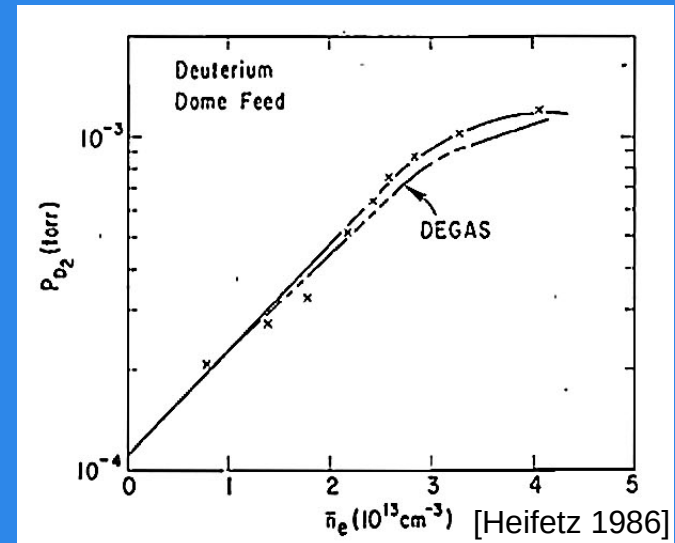
# Treatment of Elastic Scattering Recently Improved

- $\text{H} + \text{H}^+ \rightarrow \text{H}^+ + \text{H}$ ,
  - Originally handled purely as charge exchange,
  - Improved dramatically with  $d\sigma/d\Omega$  calculations by Krstic & Schultz of total elastic scattering cross section [Krstic 1998].
- $\text{H}_2 + \text{H}^+ \rightarrow \text{H}_2 + \text{H}^+$ ,
  - Elastic scattering important mechanism for momentum and energy transfer to  $\text{H}_2 \Rightarrow$  longer mfp.
  - Computed by Krstic & Schultz.



# More Recent Modeling Has Dealt with Higher Densities and Lower Temperatures in Divertor

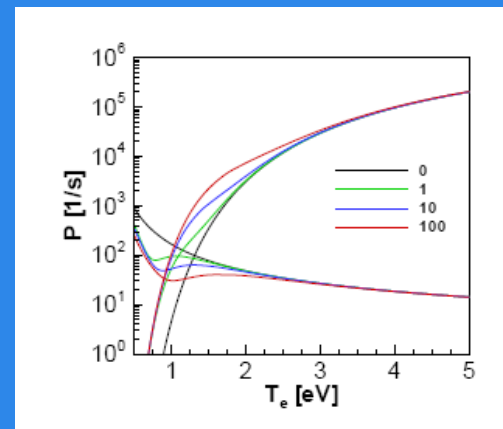
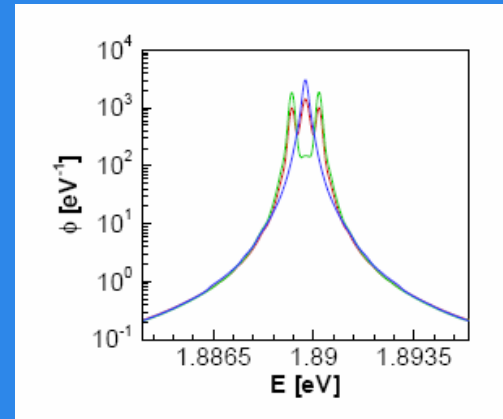
- **Viscosity of neutral gas becomes important,**
  - I.e., **neutral – neutral elastic scattering of D, D<sub>2</sub>, ( and He),**
  - D<sub>2</sub> – D<sub>2</sub> mfp = 8 cm / P<sub>D2</sub> (mTorr)
    - ⇒ High density experiments well into “transition” regime, mfp << d.
  - For ITER, P<sub>D2</sub> ~ few mTorr, d ~ 10 cm.
- **Good theoretical cross sections exist [Krstic 1998],**
  - But, handling nonlinearity requires approximate BGK description [Kukushkin 2005],
    - Rates based on empirical viscosities & diffusivities.
  - Large effect on simulated neutral pressures,
    - Again due mostly to heating of D<sub>2</sub> by D [Kukushkin2005].





# Trapping of Lyman Series Radiation

- Mean free path for Ly- $\alpha$   $\sim 0.2 \text{ cm} / n_D(10^{20} \text{ m}^{-3})$  [Post 1995],
  - $\Rightarrow \ll$  local dimensions in some present machines & in ITER.
- Modeling is extremely complex since it couples plasma  $\leftrightarrow$  neutrals  $\leftrightarrow$  radiation field,
  - Even more nonlinear,
  - Line shape effects important.
- Photon transport modeled in EIRENE with same Monte Carlo tools used for atoms & molecules,
  - And incorporates photo-excitation into H CR model [Reiter 2002],
  - Stand-alone code examining line shape effects [Reiter 2006].
  - Self-consistent B2-EIRENE model of ITER shows factor of two increase in plasma density, somewhat lower plasma temperature [Reiter 2006].
- Alternative approach: incorporate simple plasma transport model into NLTE code CRETIN [Adams 2004],
  - Used to benchmark modified CR rates [Scott 2004]  
 $S_{\text{eff}}(n_e, T_e, L)$ ,  $R_{\text{eff}}(n_e, T_e, L)$  for use in existing plasma & neutral transport codes.

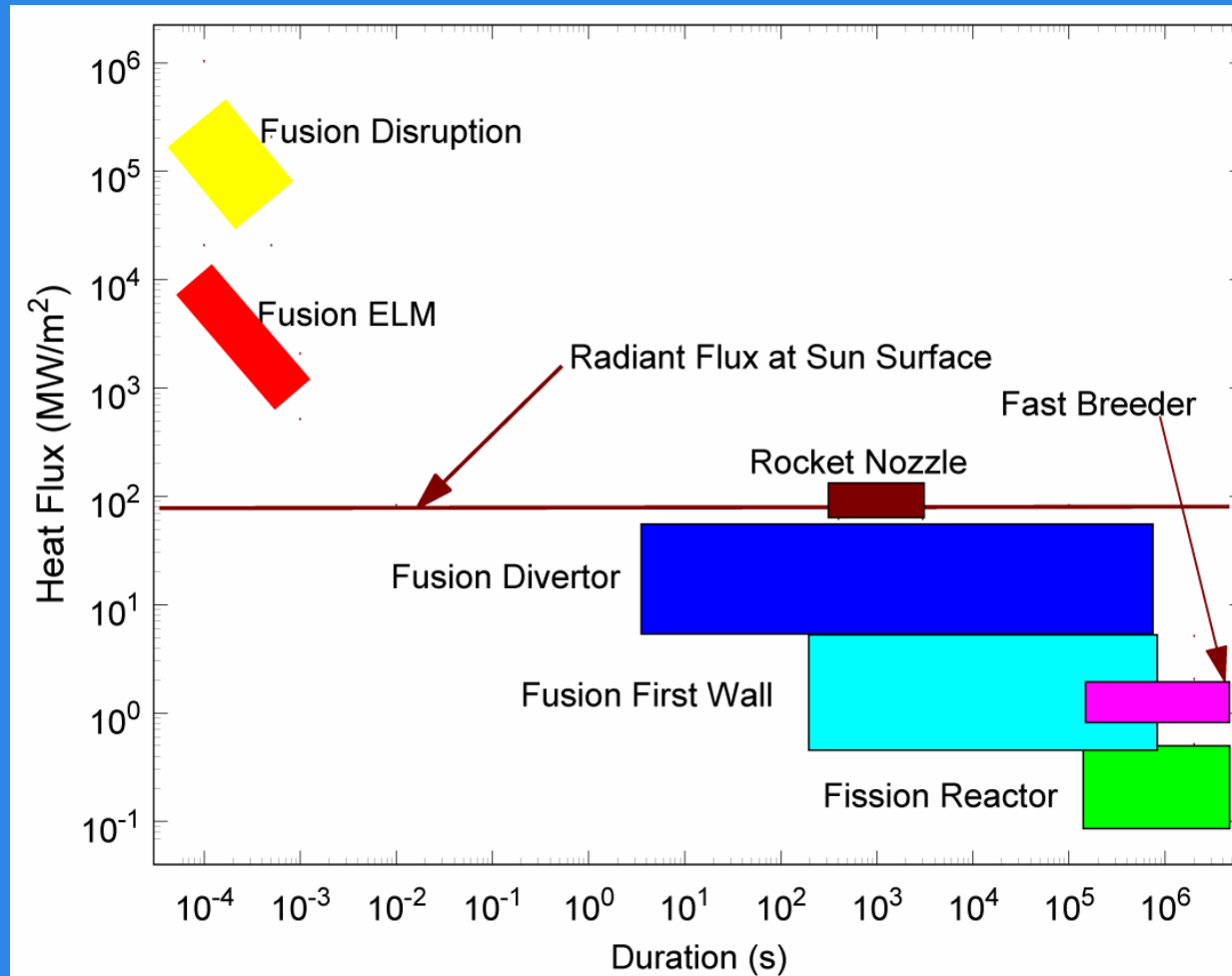


[Adams 2003]

# More Complex $\text{H}_2$ , $\text{H}_2^+$ Behavior

- Lower temperatures  $\Rightarrow$   $\text{H}_2$  lifetime extended  $\Rightarrow$  undergo additional processes,
  - Including vibrational excitation & de-excitation,
  - $\Rightarrow$  ion conversion:  $\text{H}_2(\nu) + \text{H}^+ \rightarrow \text{H}_2^+ + \text{H}$ ,
  - Also brings in other species:  $\text{H}_3^+$ ,  $\text{H}^-$ .
- Initial predictions were for “Molecule Assisted Recombination” [Krasheninnikov 1997],
  - But, ASDEX-U modeling [Fantz 2001], showed instead “Molecule Assisted Dissociation”!
  - Explicitly modeled transport of vibrationally excited molecules!
- Attempts to fold effects into effective “collisional radiative” rates for  $\text{H}_2$ ,  $\text{H}_2^+$ : [Sawada 1995, Greenland 2001, Pigarov 2002].
- [Janev 2003] reviews & assesses current data,
  - More data still needed:
    - State-selective processes involving vibrationally excited states,
    - Impact of rotational excitation on plasma kinetics,
    - Isotope specific data.
  - Sawada has more complete model on the way.
  - Still need to be integrated into comprehensive, simplified model for simulations.

# Is 60 MW/m<sup>2</sup> a Problem?



[M. A. Ulrickson, Sandia National Labs]