Fundamental surface science of PFCs for improved plasma performance in NSTX-U

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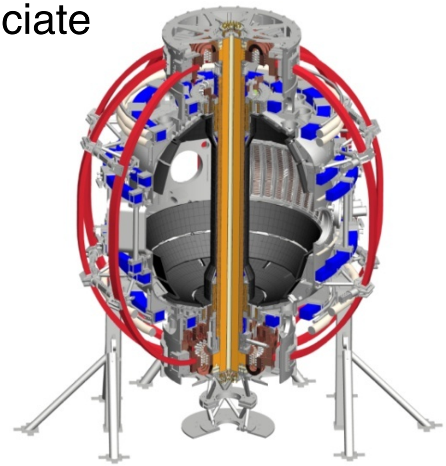

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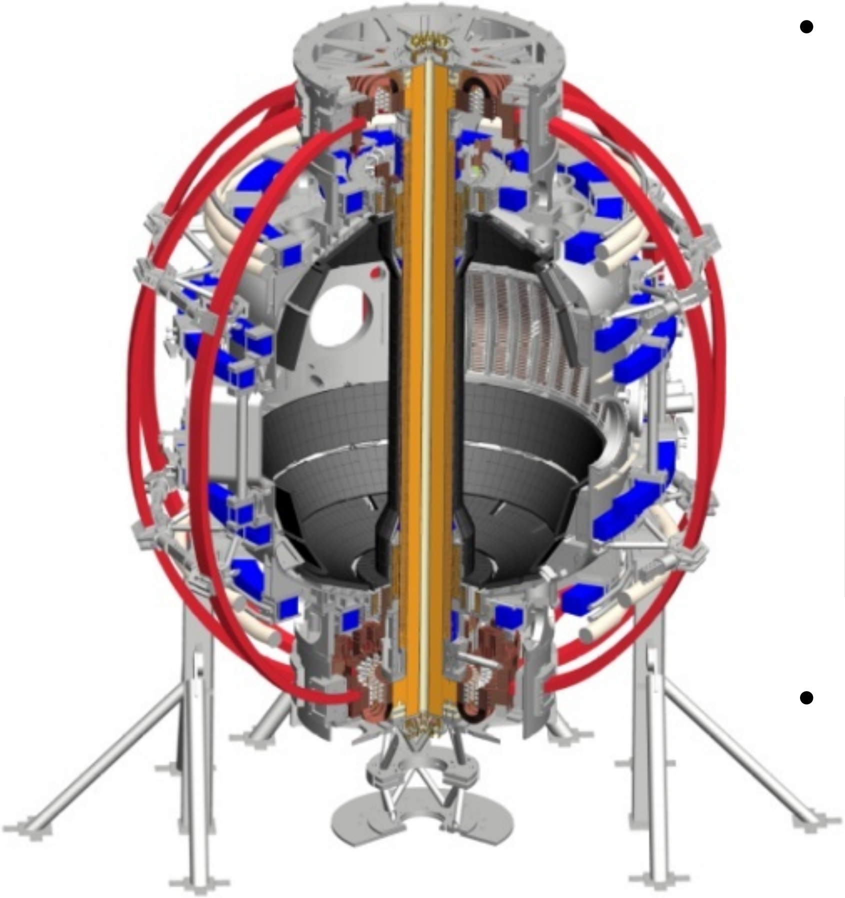
PFCs in NSTX-U



NSTX-U

pppl.gov

- PFCs in NSTX-U will have to withstand higher particle and heat loads:
  - Upgrade: double the toroidal magnetic field to 1 T, plasma current to 2 MA and the neutral beam heating power to 14 MW
  - Increase pulse length from 1 to 7 s.

➔ a better understanding of PMI processes needed for NSTX-U operations and the future development of Li-conditioned PFCs during high-heat flux long-pulse scenarios is crucial

- Materials we focus on:
  - Li-C-O-B layers (B used for PFC conditioning) (Sn and Sn-Li also)
  - Mo and TZM substrates for the gradual transition to high-Z PFCs
  - D(H) and He incident particles

Surface science for NSTX-U

- ***How will Li perform under the plasma conditions of future fusion devices (heat and particle flux, ion energy, surface temperature, etc.) in terms of:***
  - ***H isotope intake***
  - ***Impurity segregation***
  - ***Evaporation (operational temperature range)?***

- Understanding PMI processes:
  - D retention in Li films as a function of impurity level (C, O) and surface temperature (on Mo substrates)
  - Boron and Lithium conditioned plasmas performance, D retention and surface chemistry in Mo-B-O-C and Mo-Li-O-C layers: *a comparison with MAPP results*
  - Diffusion coefficient of O in Li and its temperature dependence; developing strategies for the removal of contaminants
  - Li and Sn wetting of TZM; Investigations with TPD to determine Li-Mo and Sn-Mo adhesion energies
  - Composition and surface chemistry of Sn and Sn-Li alloys for alternative PFC solutions
    - Thermally induced segregation mechanisms of Sn-Li alloys
    - D retention in Sn and Sn-Li alloys
  - D^+ sputtering coefficients of Li and Li-C-O layers

Experimental approach

Surface Science and Technology Laboratory, SSTL (T260)
Surface Imaging and Microanalysis Laboratory, SIML (C123)
Laboratory for Surface Chemistry (PU)

- ***Spectroscopy – Surface composition, structures***
  AES, HRXPS, XPD, LEIS, ALISS, UPS, HREELS, ELS, ESD, $\Delta\varphi$, LEED, RHEED, SEE measurement
- ***Mass separated mono-energetic ion beam***
  Colutron ion gun (Tectra plasma source)
- ***Surface imaging***
  SAM, SEM, STM
- ***Deuterium retention***
  TPD

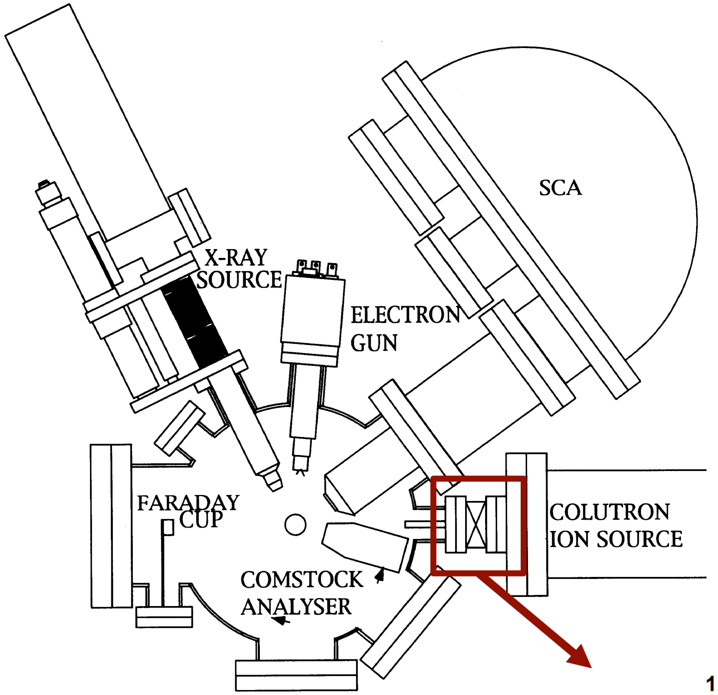
Laboratory experiments have many advantages

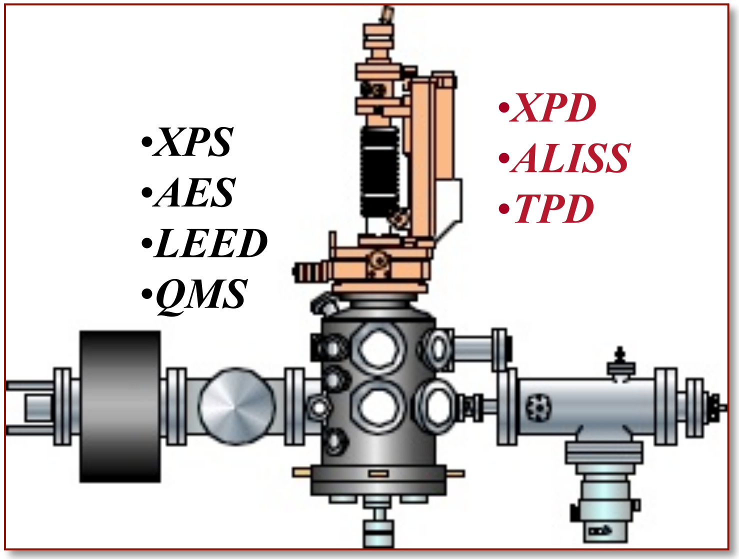
Fusion experiments occur in challenging conditions for understanding PMI processes:

- Technical difficulties for performing *in-situ* analysis
- Complex environment in terms of characterization of the plasma parameters, particle species, energies, fluxes, sample temperature, *etc.*

- Lab experiments allow simulating materials and coatings in a controlled way and understanding the fundamental physics and chemistry occurring at surfaces
- It is possible to utilize surface sensitive analysis techniques and directly follow the surface chemistry
- Well-characterized ion beams in terms of energy and ion species
- Thin film layers can be deposited in a controlled way on various substrates

XPS/XPD/LEIS/ALISS instrument

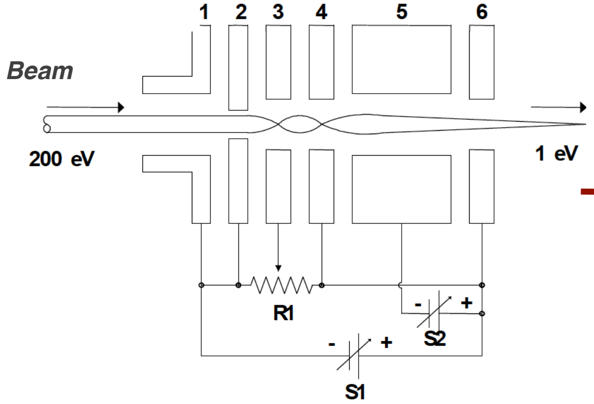


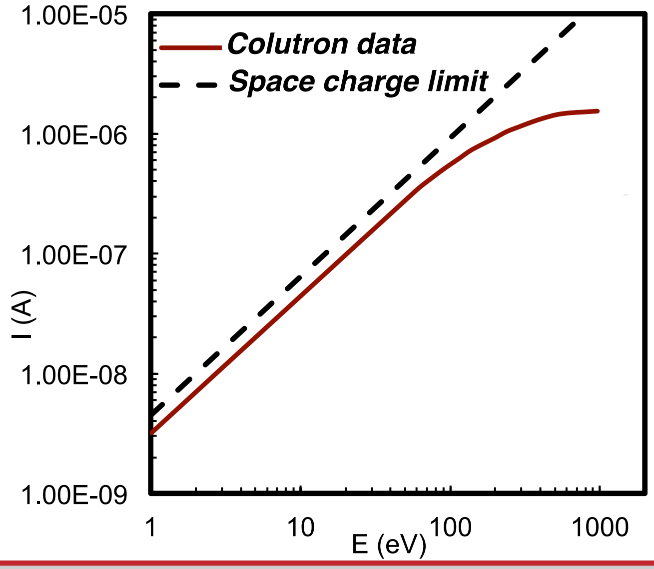


- *XPS*
- *AES*
- *LEED*
- *QMS*

- *XPD*
- *ALISS*
- *TPD*

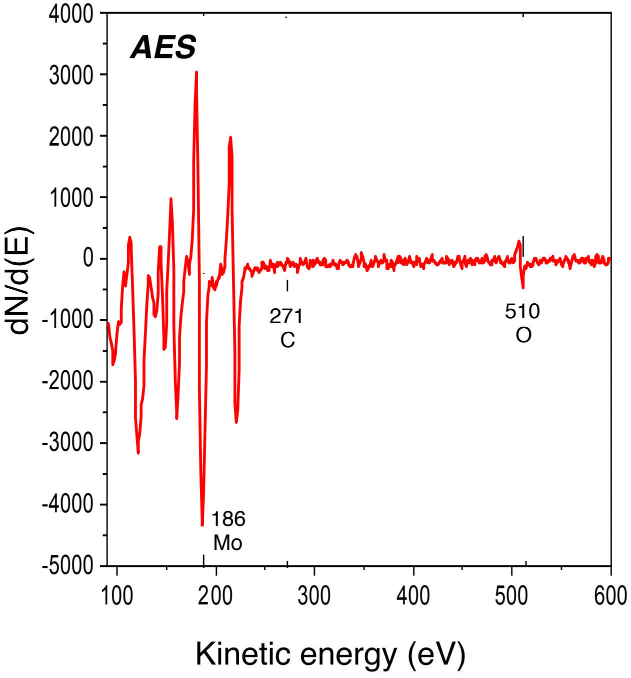
Deceleration system

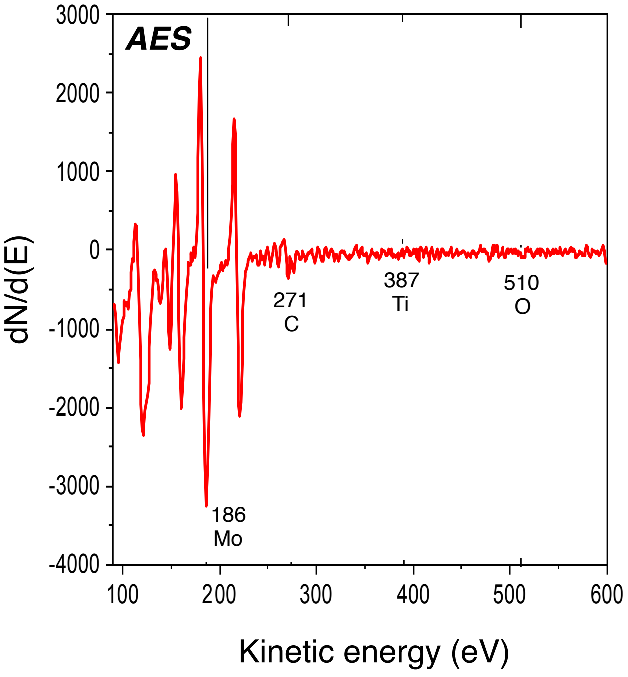


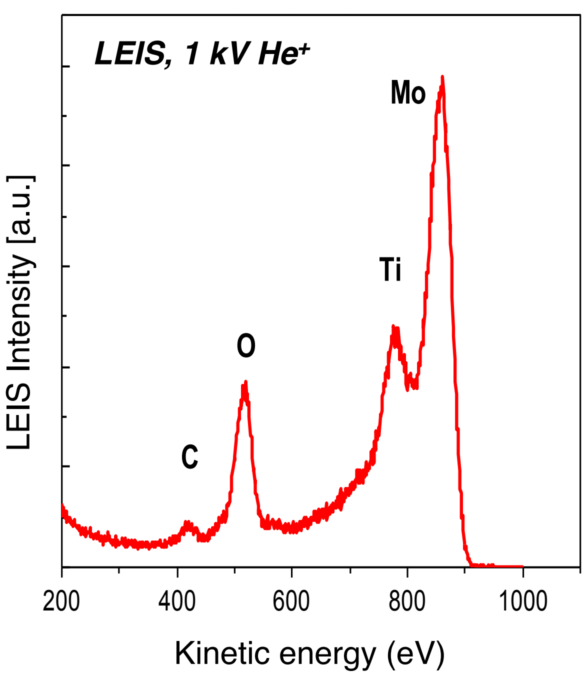


Model 400 deceleration lens mounted at the exit of ion gun, consisting of six electrically insulated concentric cylinders

Well-defined surfaces: AES & LEIS analysis

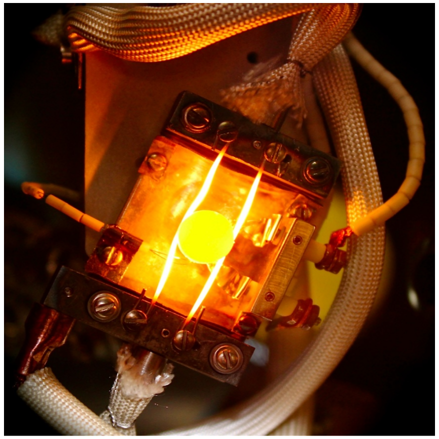

Mo(poly)


TZM


TZM

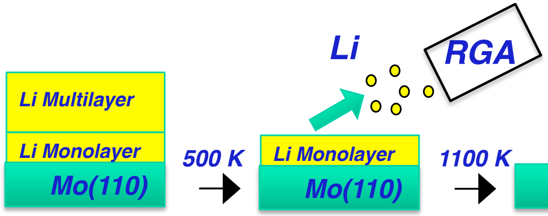
- **Ar⁺ ion sputtering and high temperature annealing (1800 K) was used to prepare clean surfaces for experiments, as probed by AES and LEIS analysis**
  - **Mo(poly) surface has 6% O; TZM surface has 2% C, no Ti**
  - **After extensive oxidation and annealing, LEIS shows Ti and O on the TZM surface**

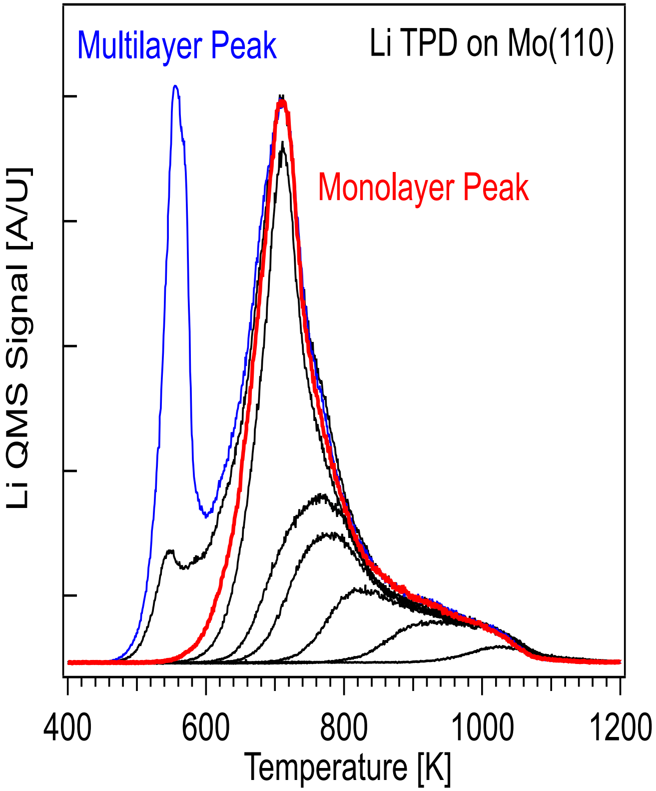
TPD: thermal stability of Li on Mo(110) and D retention

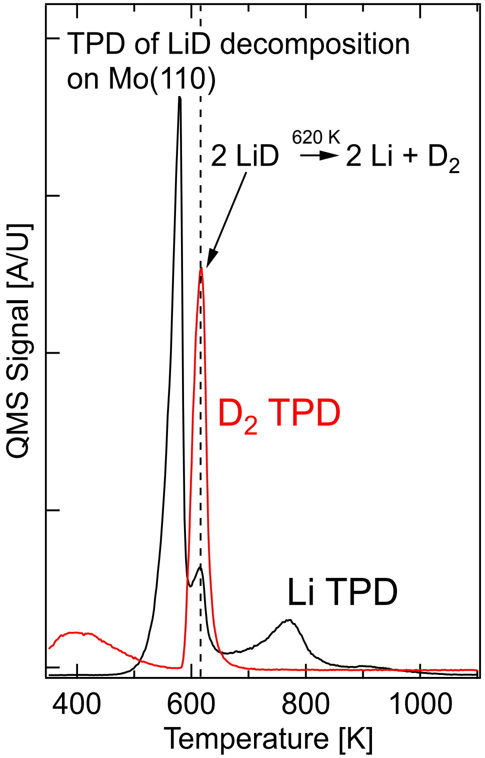


Mo(110) resistively heated in UHV

- ***Temperature Programmed Desorption (TPD) used to study Li films and D retention***
- ***Sub-monolayer control of film thickness and D flux***
- ***Area under TPD curve is proportional to atomic concentration desorbed***
- ***Desorption peak temperatures correlated with binding (adsorption) energies***





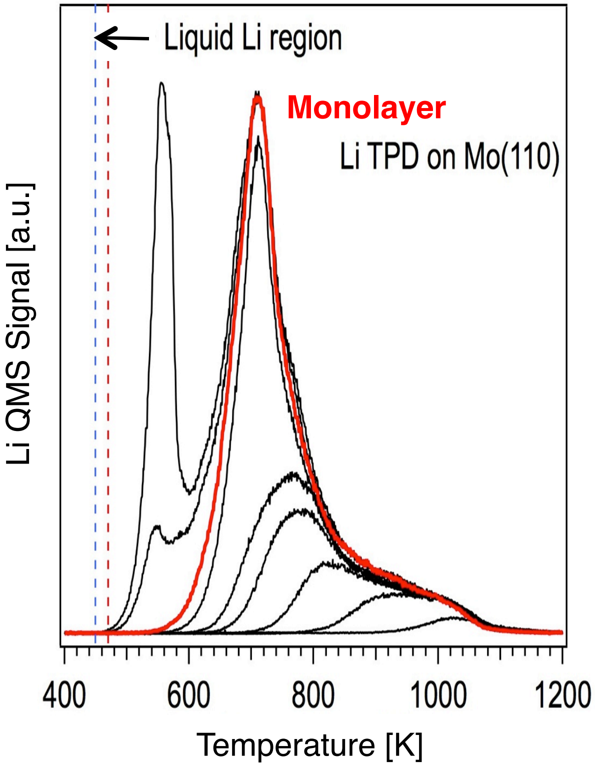


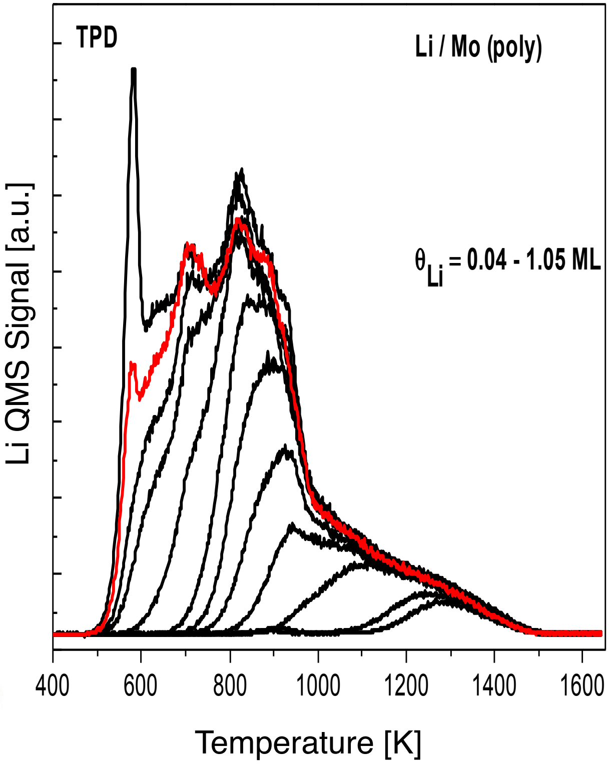
Chen, Roszell, Scoullos, Riplinger, Koel, Carter, *J. Phys. Chem. B*, Article ASAP

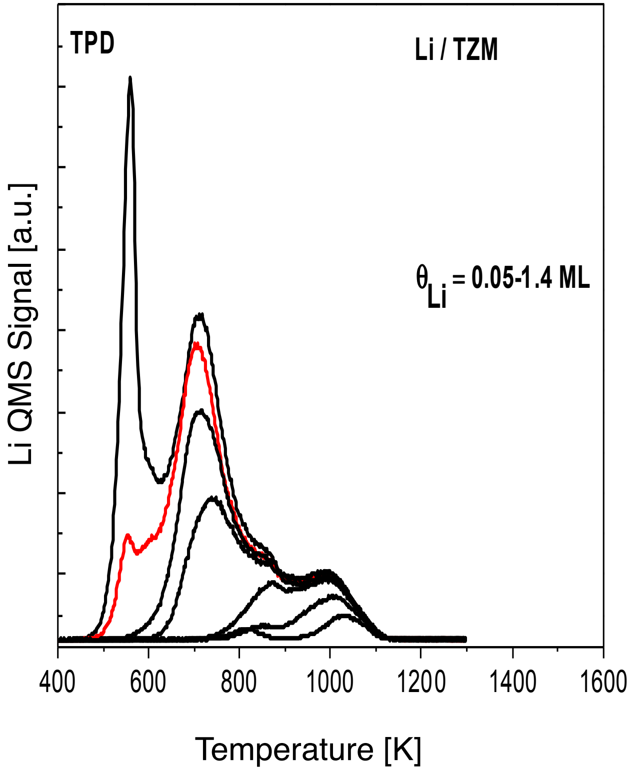
Capece, Roszell, Skinner, Koel, *J. Nucl. Mat.*, 463, 1177 (2015)

Roszell, Capece, Koel, *SOFE 2015*

Thermal stability of Li on Mo substrates



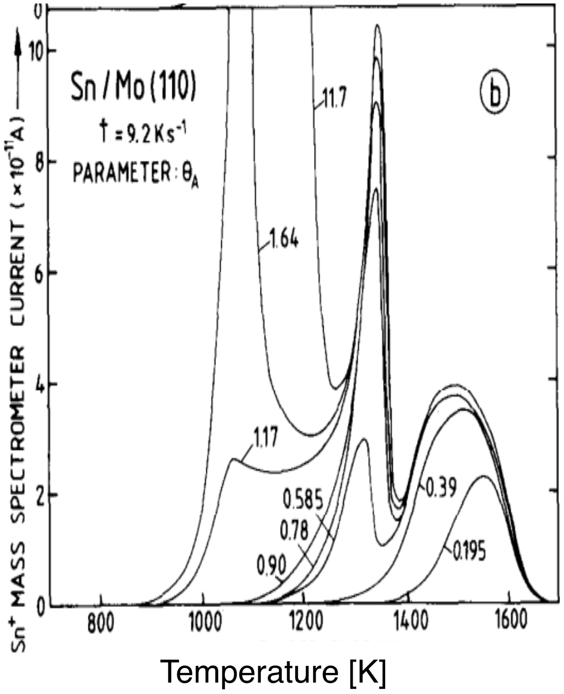


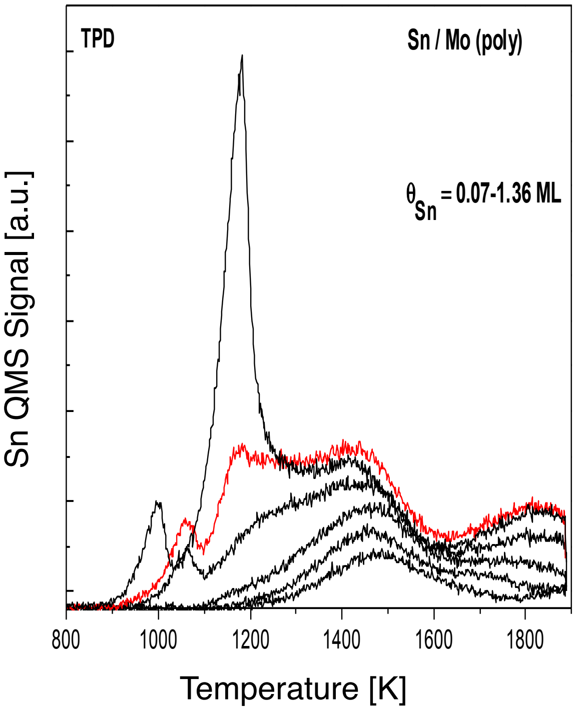


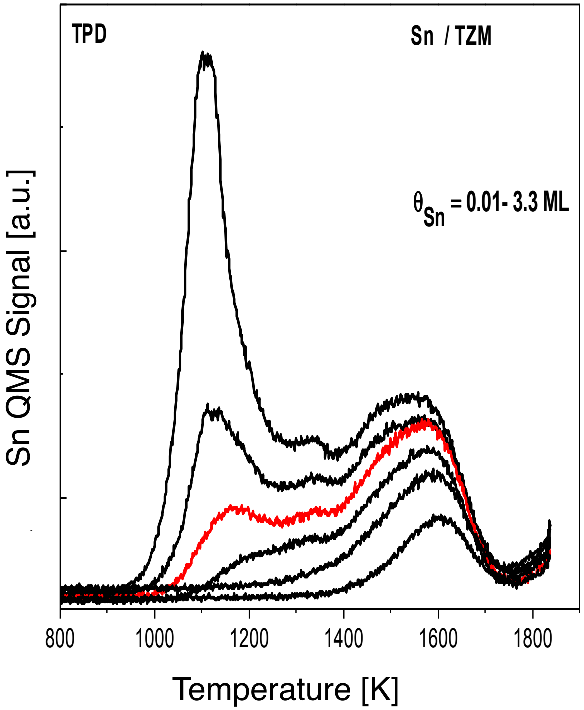
- **m.p.(Li) = 180 °C (453 K)**
- **Li multilayers (thick films) start to desorb at 465 K**
- **On Mo(110) and TZM, Li is fully desorbed, completely removed, at 1100 K**
- **On Mo(poly), Li is more stable and remains at surface up to 1500 K**

Chen, Roszell, Scoullos, Riplinger, Koel, Carter, *J. Phys. Chem. B*, Article ASAP

Thermal stability of Sn on Mo substrates





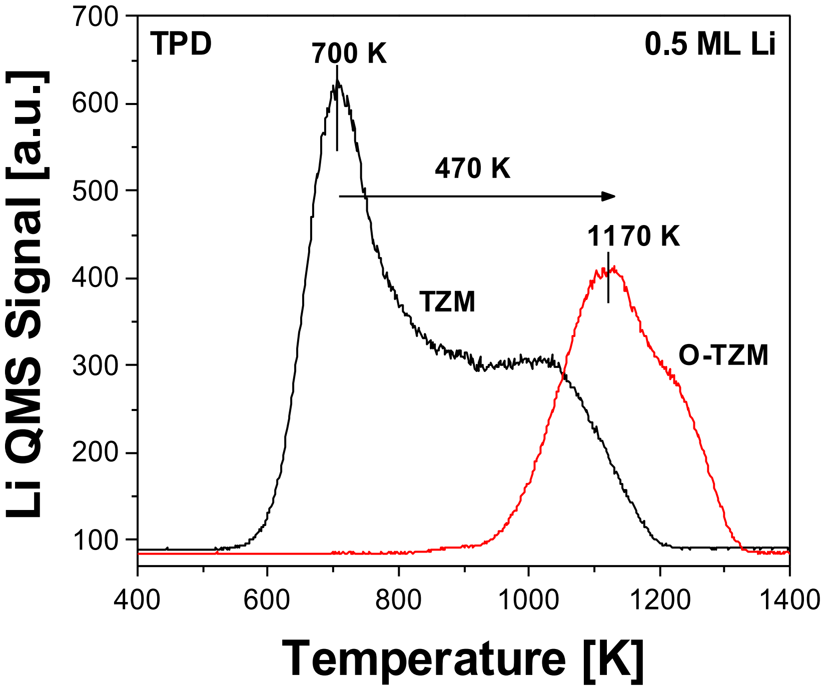


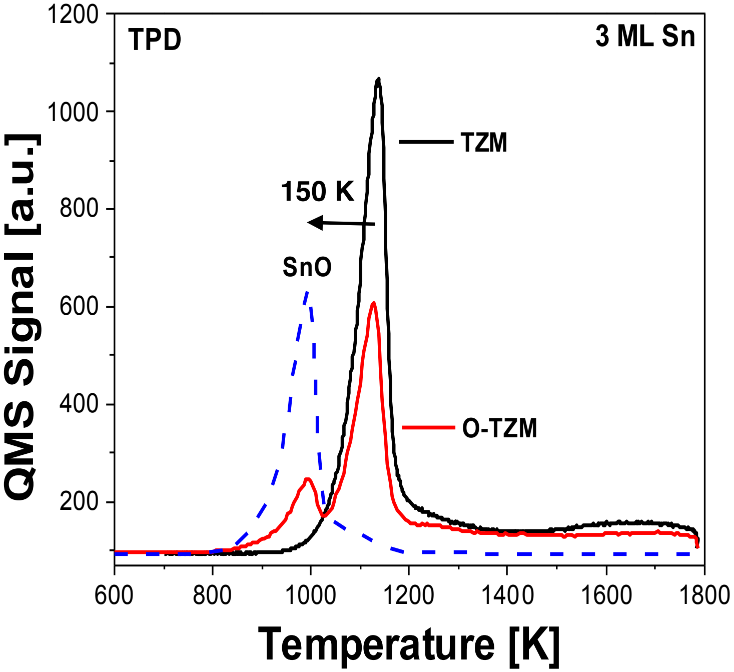
- **m.p.(Sn) = 232 °C (505 K)**
- **Sn multilayers (thick films) start to desorb at 900 K**
- **SnO forms from interaction with O impurities, and desorbs at lower temperature than Sn thick films**
- **Sn monolayer film is stable up to temperatures of 1700 K on Mo(poly) and TZM**

M. Tikhov, E. Bauer, *Surf. Sci.* 203 (1988) 423

Oxidation/contamination of TZM has different effects on Li and Sn thermal stability

Oxidation of TZM produces surface that is
81% Mo, 7% Ti and 13% O: TiO_2/Mo

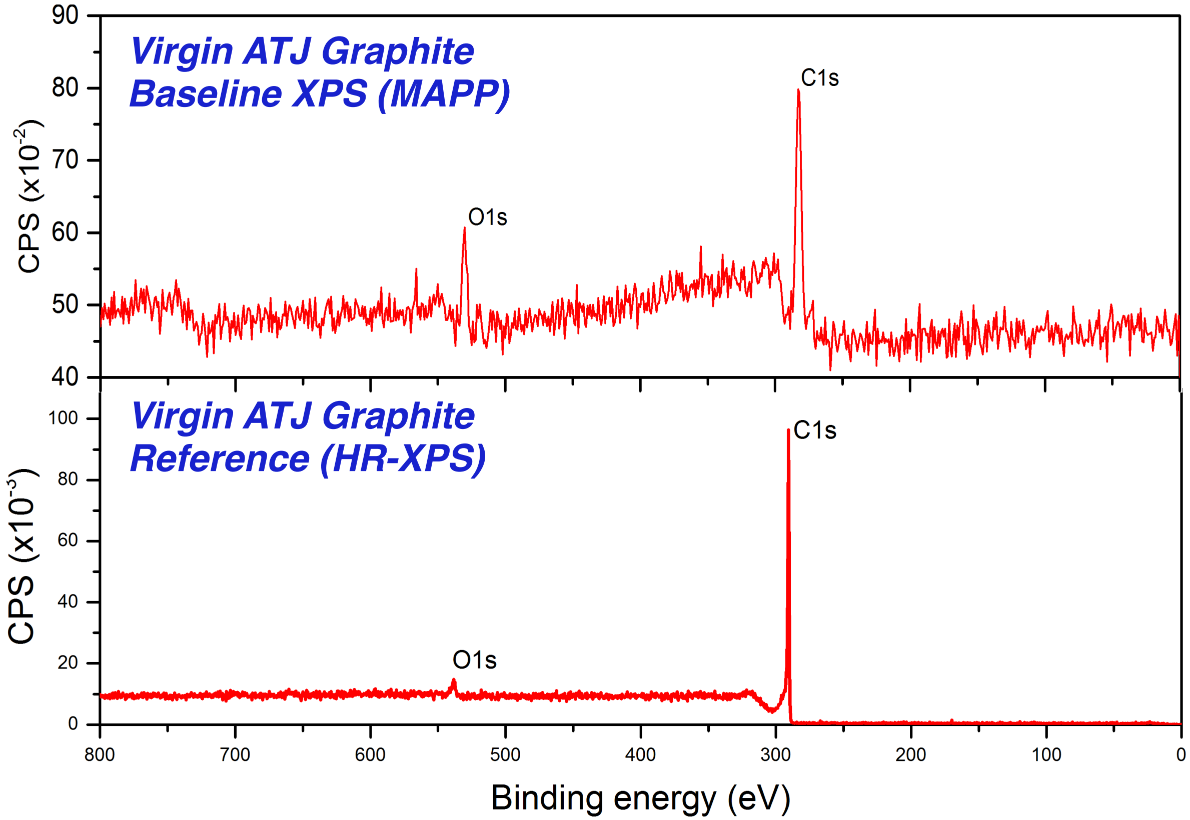


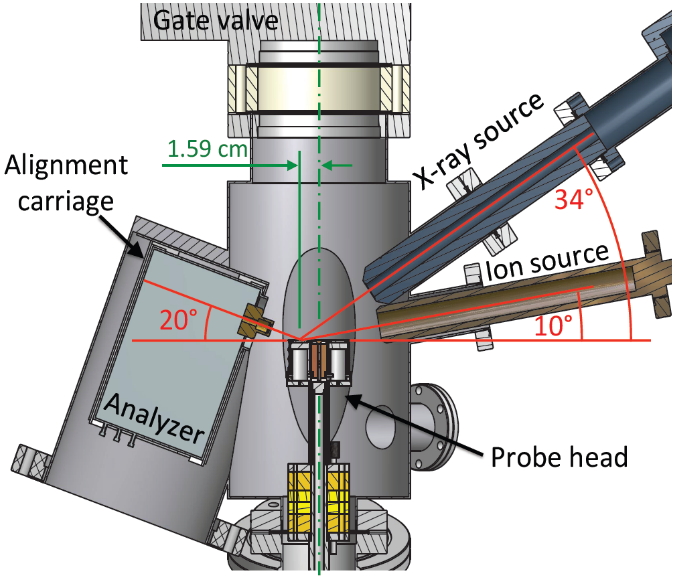


- **Li and Sn deposition on oxidized TZM surface forms Li_2O and SnO**
- **Li_2O is more thermally stable and exhibits lower Li v.p. than Li films**
- **SnO has higher v.p. than Sn films and desorbs below 1000 K**

Surface spectroscopy to complement MAPP analysis

High-resolution XPS of ATJ samples provides the basis to analyze and benchmark XPS data from MAPP



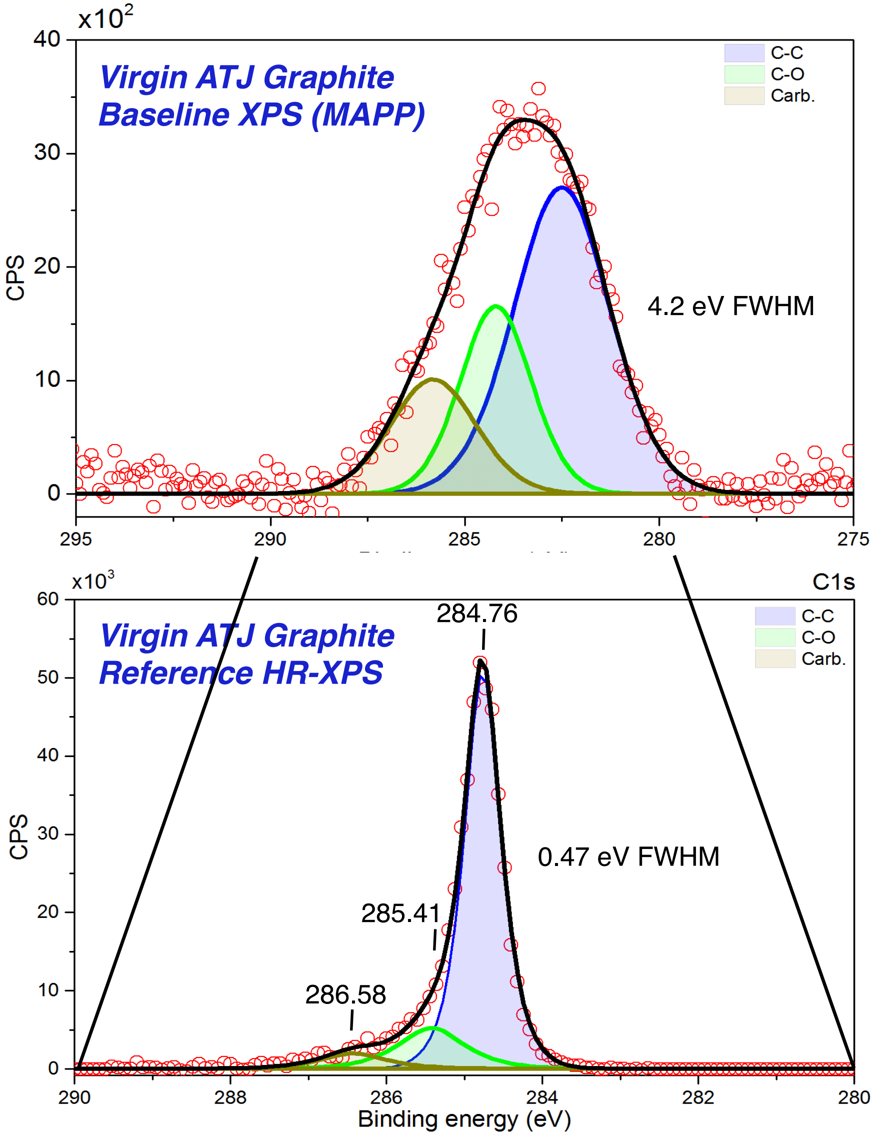


MAPP probe

Samples can be taken for additional studies to SSTL or SIML at PPPL or to Princeton University after removal from MAPP

F. Bedoya, *et al.*

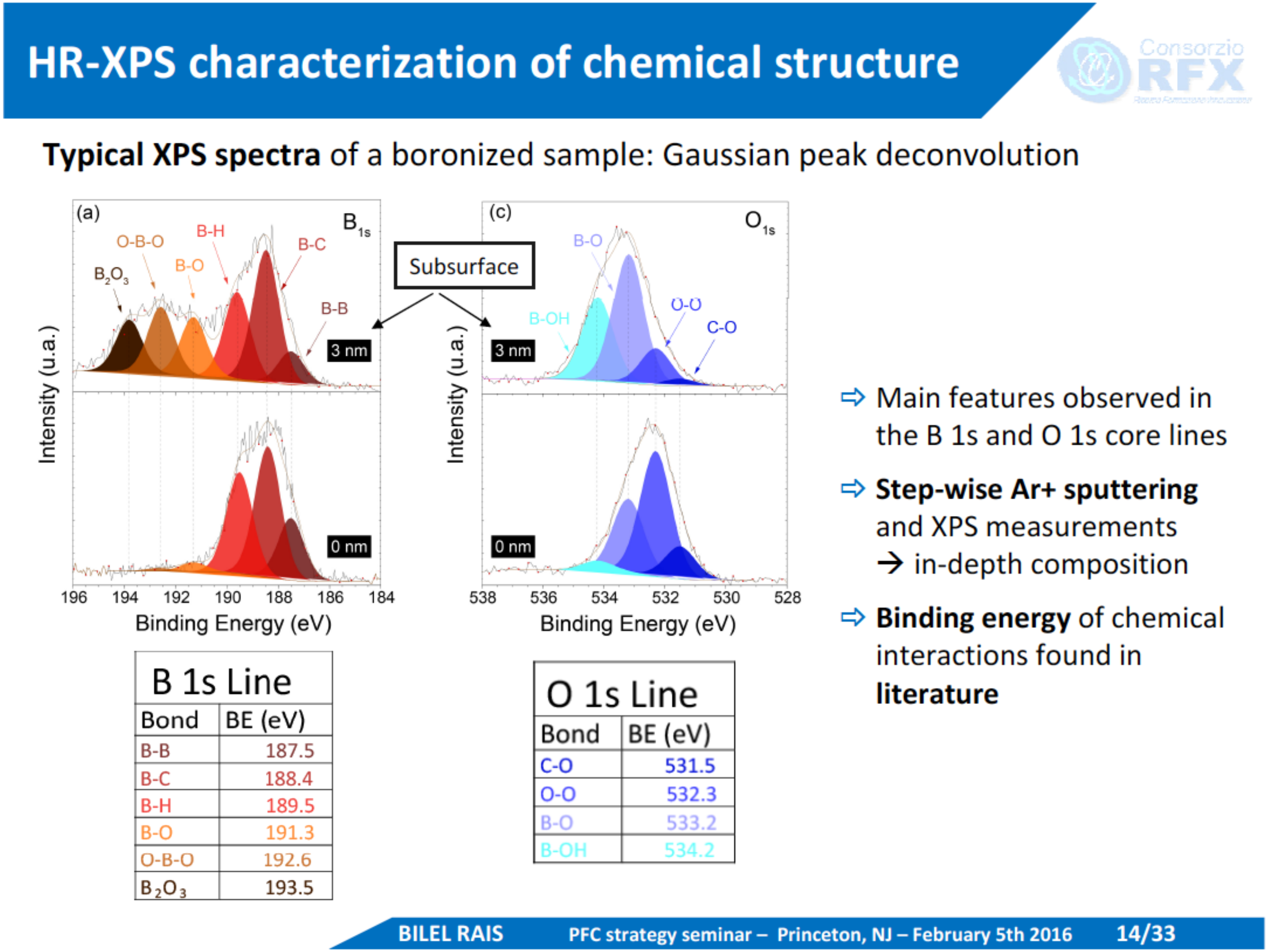
HR-XPS and the assignments in MAPP spectra



The identity, number, and concentration of surface species, i.e. peaks in each region, can be identified using reference spectra obtained by HR-XPS

F. Bedoya, *et al.*

Helping to unravel the effect of boronization wall conditioning on plasma performance



HR-XPS characterization of chemical structure

Typical XPS spectra of a boronized sample: Gaussian peak deconvolution

B 1s Line	
Bond	BE (eV)
B-B	187.5
B-C	188.4
B-H	189.5
B-O	191.3
O-B-O	192.6
B_2O_3	193.5

O 1s Line	
Bond	BE (eV)
C-O	531.5
O-O	532.3
B-O	533.2
B-OH	534.2

⇨ Main features observed in the B 1s and O 1s core lines

⇨ **Step-wise Ar+ sputtering** and XPS measurements
→ in-depth composition

⇨ **Binding energy** of chemical interactions found in **literature**

BILEL RAIS PFC strategy seminar – Princeton, NJ – February 5th 2016 14/33