Studies of lithiumization and boronization of ATJ graphite PFCs in NSTX-u

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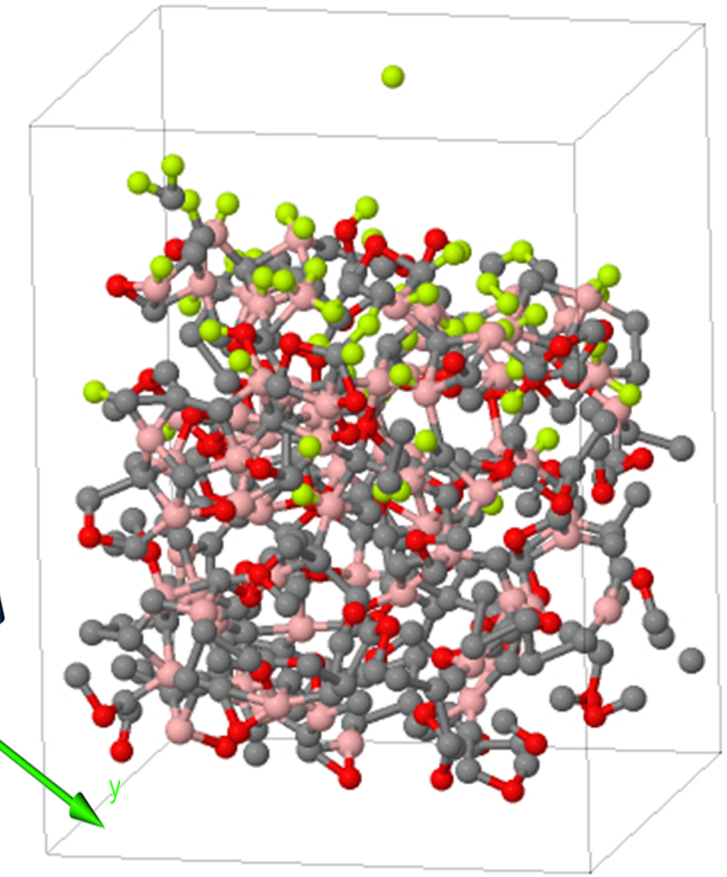
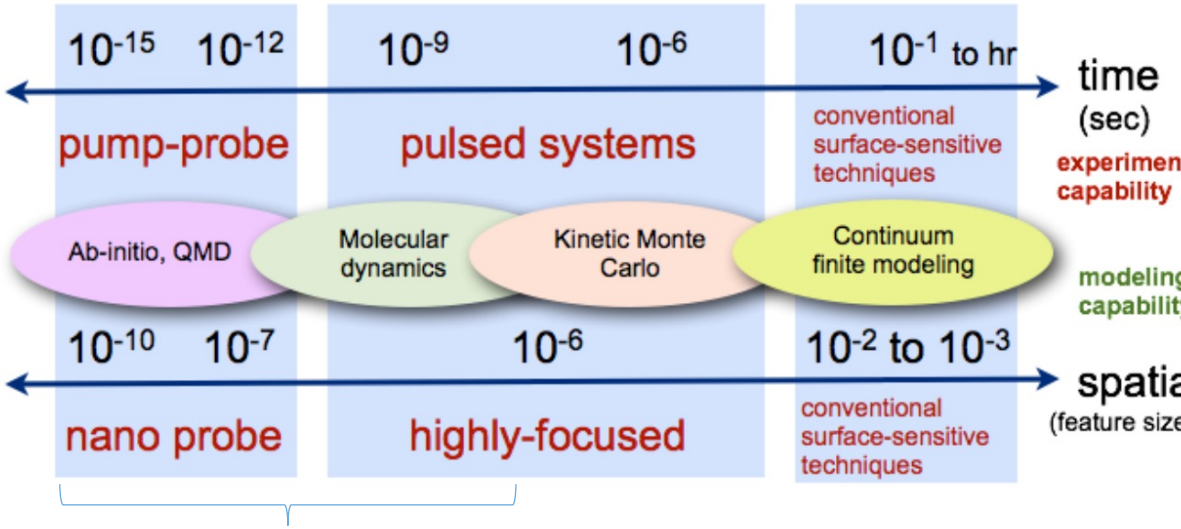
re we doing?

culate chemistry, retention of D, chemical sputtering of a B-C-O-D, Li-C-O-D and B-Li-C-O-D surface.

To understand the fundamental processes in the windows of time&space when these actually happen.





Here we are: atomistic approaches

Most processes end in less than 100 ps . Cumulative process require longer time.

Flux: $10^{25}m^{-2}s^{-1}$ means I D atom at 10 nm^2 each 10 ns. Howe impact atom changes the target surface – the dynamical surf

How do we do it?

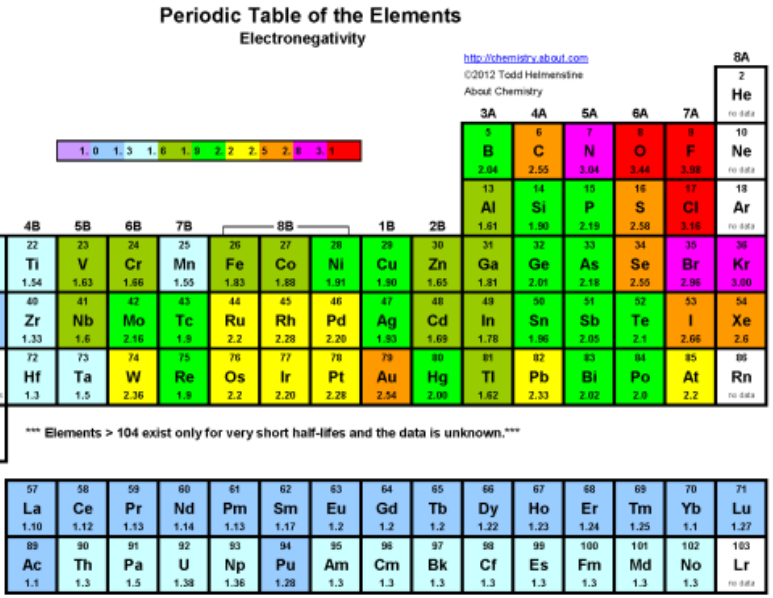
Classical molecular dynamics with REAXFF

Verified by quantum-classical molecular dynamics (need exo computing resources

Validated by NSTX-U and lab experiments whenever availabl

s classical mechanics not good for the problems with B-Li-C-O-D.?
ood for W-D or C-D problems.

The answer lays in different electronegativity of the atoms in B-Li-C-O-D m



This means polarization and charges of the atoms in mixture dynar change with change of the coordinates of atoms, in particular dur the D impact cascade. Changes in electronic cloud can be handled only by quantum mechanics.

We use **SCC-DFTB approximation to DFT which** is nominally about Times faster than DFT, still 1000 times slower than classical mecha

REAXFF: Intermediate solution: combination of classical mechanic semi-empirical QM calibrated method (**Electronegativity Equalizat** which recalculate charges each time step of classical mechanics. Th about 100 times slower than classical mechanics.

ncertainty propagates through scales?

ese computational codes have limits, so do the experimental and metrology tools. Key is to fill the ga he other and identify regions of validation in combination with the data uncertainty and more importa

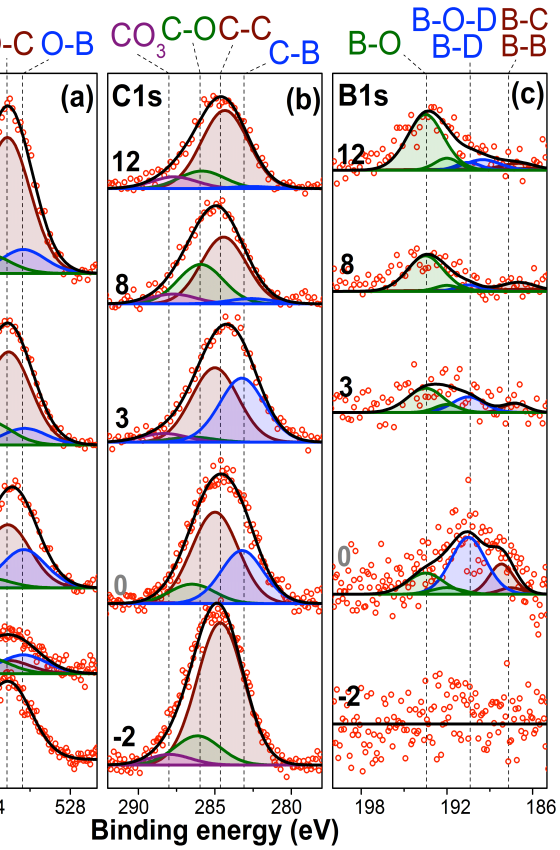
tify appropriate and strategic problems to solve

amples of the problems for NSTX-U that can swered by atom.theory validated by experime

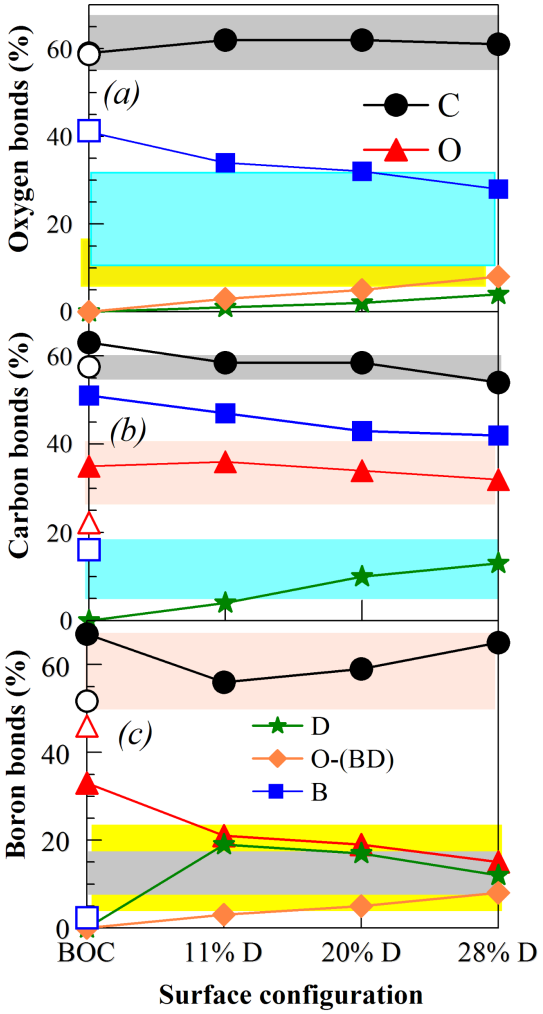
fects of B and Li deposited onto the carbon tiles. In particular:
ffects of deuterium accumulation
ffects of varying concentration of B and Li DO
deuterium retention and chemical sputtering of the surface.
pare with experimental data form MAPP and lab.
fects of impurities, in particular of O and its derivate (O_2, H_2O) at D recycling and e
uid Li on carbon and high-Z substrates. Compare with experimental data. IN W
etermine intermolecular interactions of liquid metals (Li, Sn, Ga) with high-Z subst
model the wetting.
fects of temperature and impurities on the wetting of the liquid metals, as well as
ping and release. LAT
o feed the mesoscopic dynamics (KMC) with the obtained atomistic data and to
nuum dynamics through XGC-DEGASII.

ome achieved results

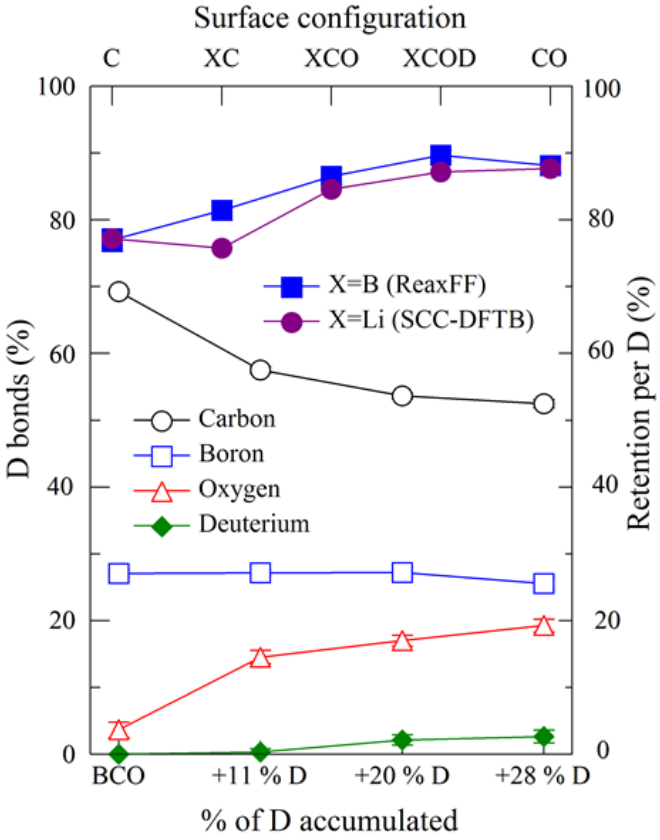
g and retention chemistry in boronized and oxidized surfaces



(b) C1s, and (*c*) B1s XPS spectra
APP with boronized ATJ graphite
s days of deuterium plasma
.

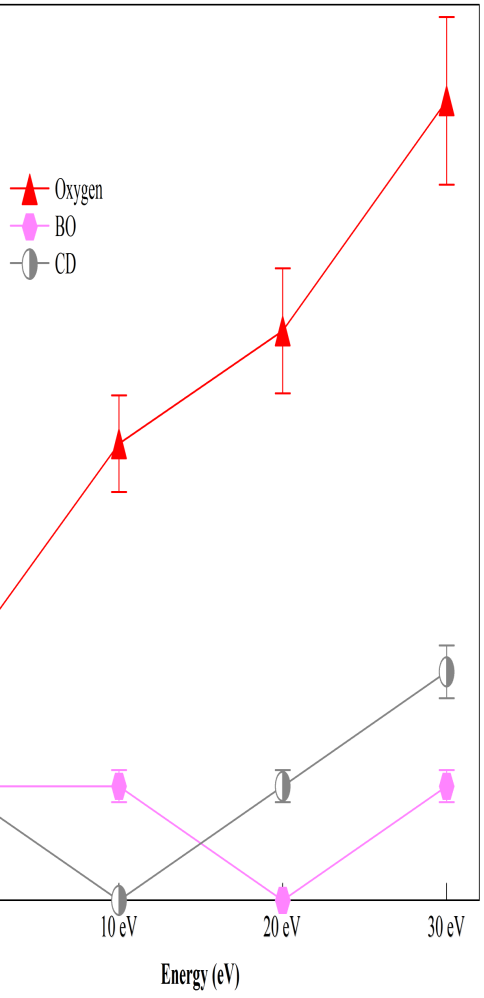


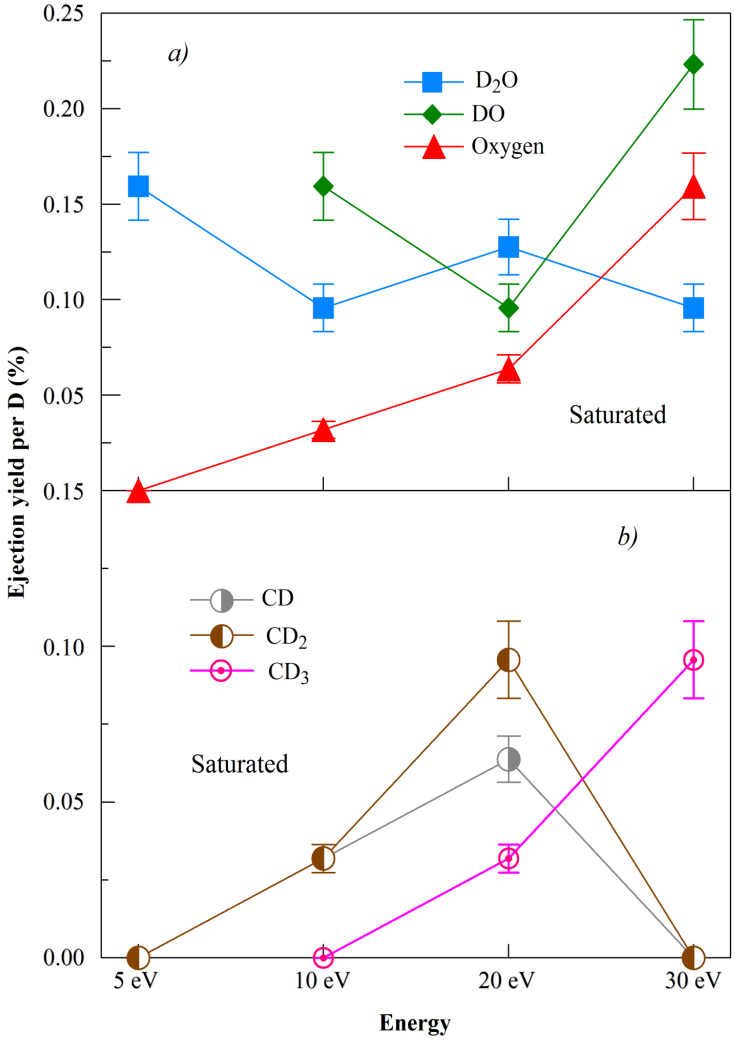
Bonds of (a) O, (b) C, and (c) B to other constituents in the BCOD as a function of D concentration.



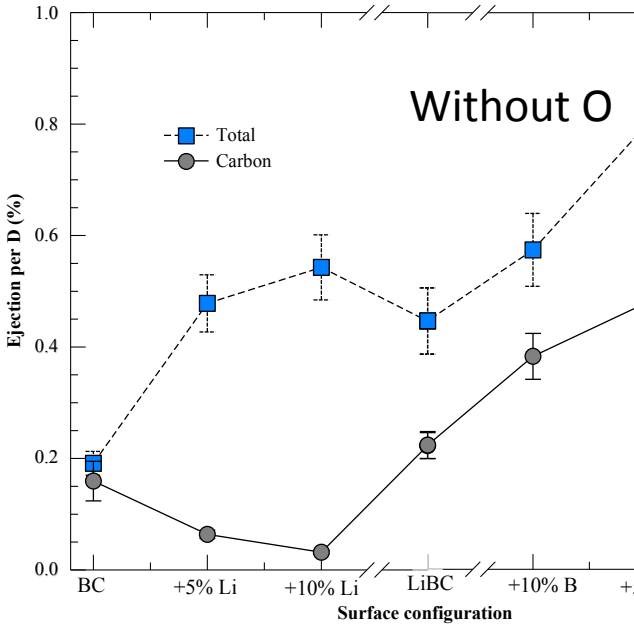
Percentage of D bonds with constituent of the deuter-ated BCO surface as function of D accumulated con-centrati (left axis). Total retention per impact of (%) on BCOD and LiCOD (right axis).

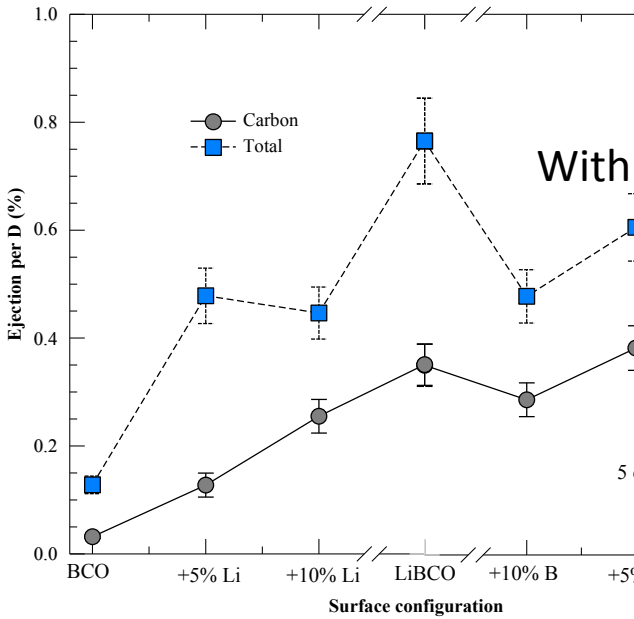
uttering of BCO as function of D impact energy





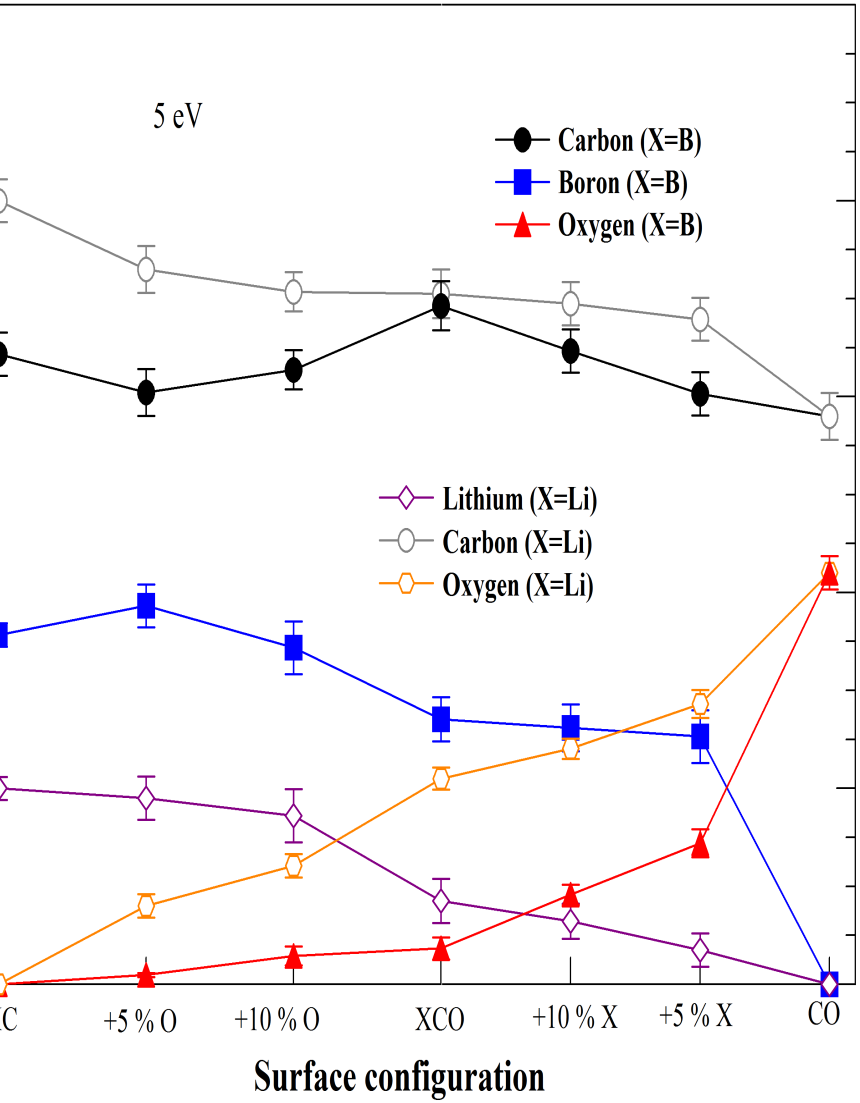
Sputtered molecules, upon D saturation



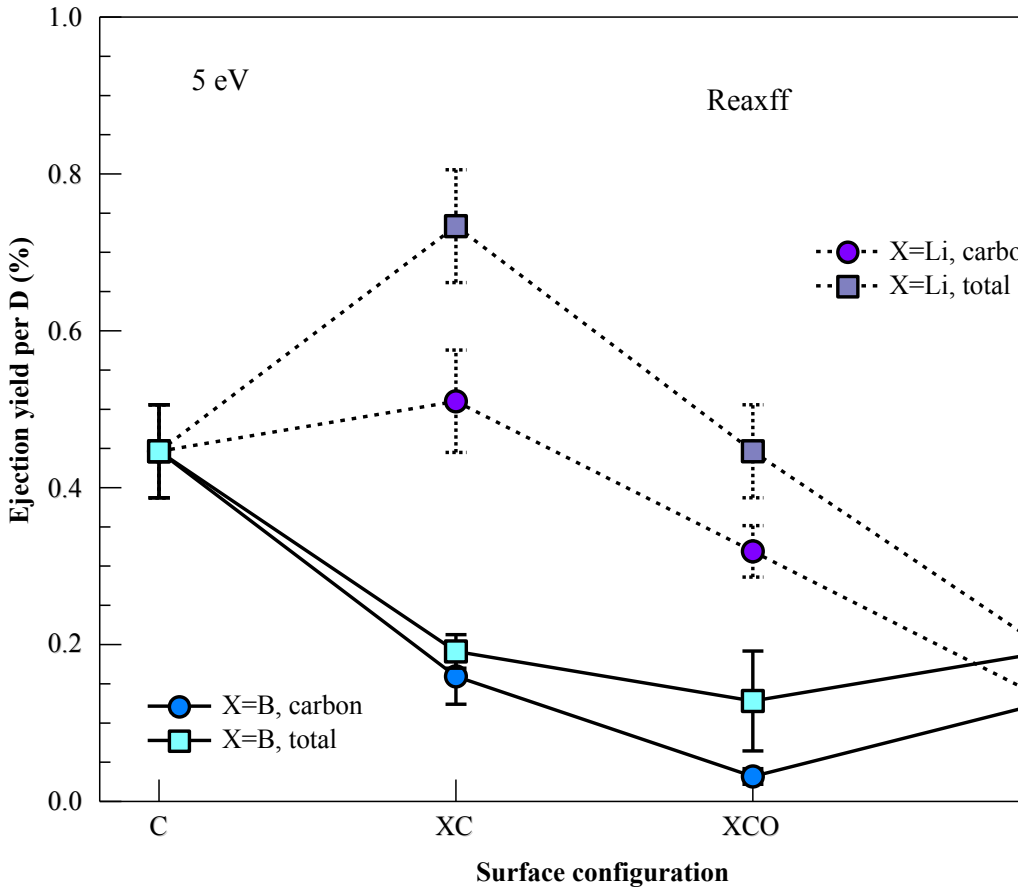


Sputtering in various configu

nparison of retention chemistry and sputtering in lithiated and boronized surfaces



ding of D to various constituents of the surface.
cumulative case at 5 eV D.



Total and C ejection yield per D for various sur
configurations

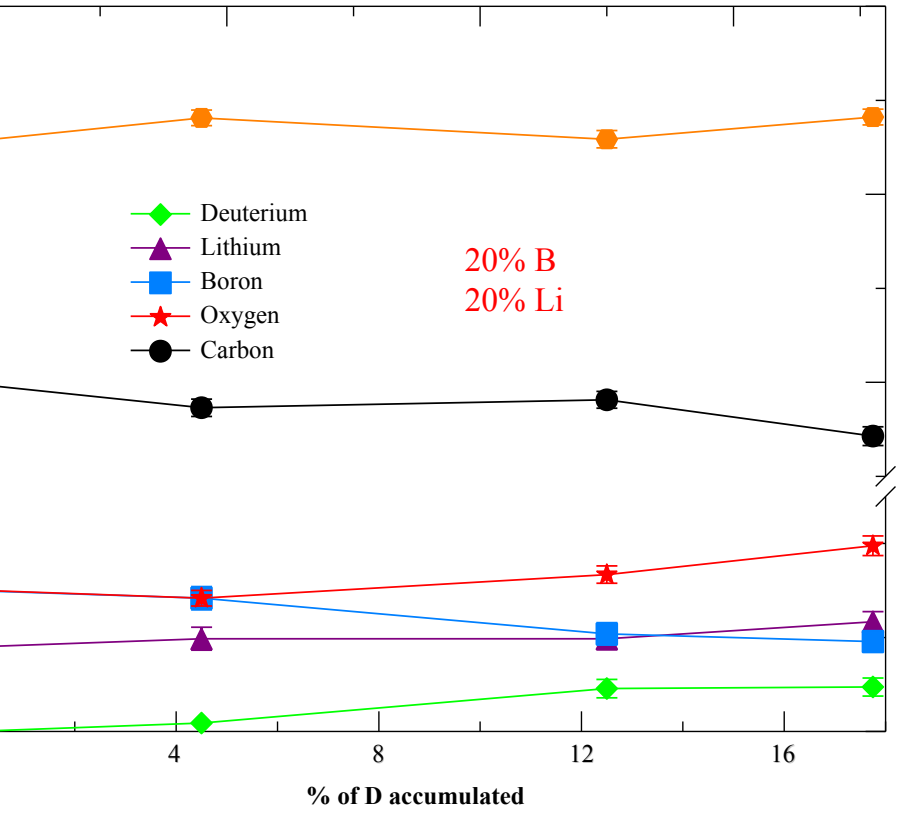
CONCLUSIONS: Outlook forward

I chemistry in NSTX-U requires QM in form of QCMD or advanced CMD+QM combinations to describe correc
gen retention and erosion in PMI.
ximate QM is adequate, however this has to be evaluated to tens of thousands of trajectories for reducing
ical error and even for correct phenomenology.
with QM over DFT for PMI systems might be not feasible in next 10 years systems.
proved classical potentials, based on multiple neighbor QM calculations are the key for next phase of the NST
stic modeling research, especially for metals. Checking DFT-fitted potentials by the methods of quantum
utational chemistry beyond DFT is doable with current computational power, leading to acceptable results, w
mental verification= Quality control.
cessing speed for extension of atomistic MD to longer times, meeting mesoscale. Algorithmic development.
nging together the various scales of PMI and plasma is the fundamental multisdisciplinary questio
ing plasma science, surface science, atomic physics, computer science and applied mathematics.
e main weight in the science of integration of fusion plasma and its interfacial surface boundaries i
MI because 1) the basic PMI phenomenology evolves much faster than the plasma time scale, and
volves through wider range of the scales, which partially overlap with the scale of plasmas.
MI has to be understood and parameterized at nanoscale before integrating it with plasma at the
e footing" at micro---scale.

Thank you!

SUPPLEMENTAL

ention chemistry and sputtering for Li-B-C-O-D



This is material mix of 5 constituents

5 eV impact of D

Oxygen gets dominant in retention chemistry (over B) once there is D accumulated