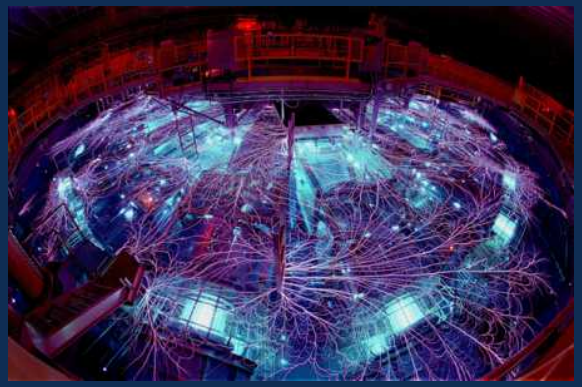
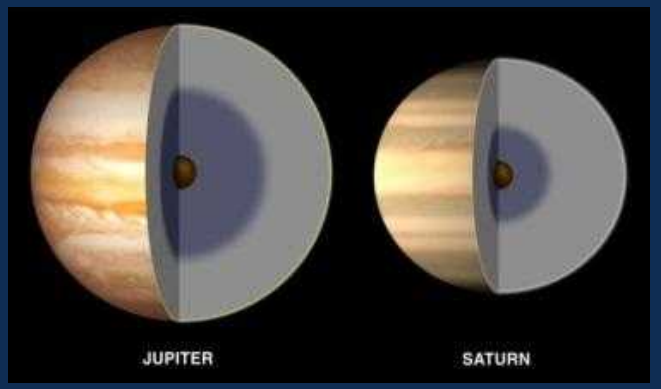
SAND2016-9359C

Exceptional service in the national interest

Sandia National Laboratories





Dynamic compression experiments on deuterium and their implications for first-principles theory

Marcus D. Knudson

mdknuds@sandia.gov / mknudson@wsu.edu

Dynamic Material Properties Group
Sandia National Laboratories
Albuquerque, NM

Institute for Shock Physics
Washington State University
Pullman, WA

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Acknowledgements

Experiment Design/Analysis

Marcus Knudson

Ray Lemke

Kyle Cochrane

Devon Dalton

Dustin Romero

Diagnostics

Charlie Meyer

Jeff Gluth

Devon Dalton

Anthony Romero

Dave Bliss

Alan Carlson

QMD Calculations

Mike Desjarlais

Andreas Becker

Winfried Lorenzen

Ronald Redmer

Planetary Modeling

Nadine Nettelmann

Andreas Becker

Ronald Redmer

Pulse Shaping

Ray Lemke

Jean-Paul Davis

Mark Savage

Ken Struve

Keith LeChien

Brian Stoltzfus

Dave Hinshelwood

Entire Z crew

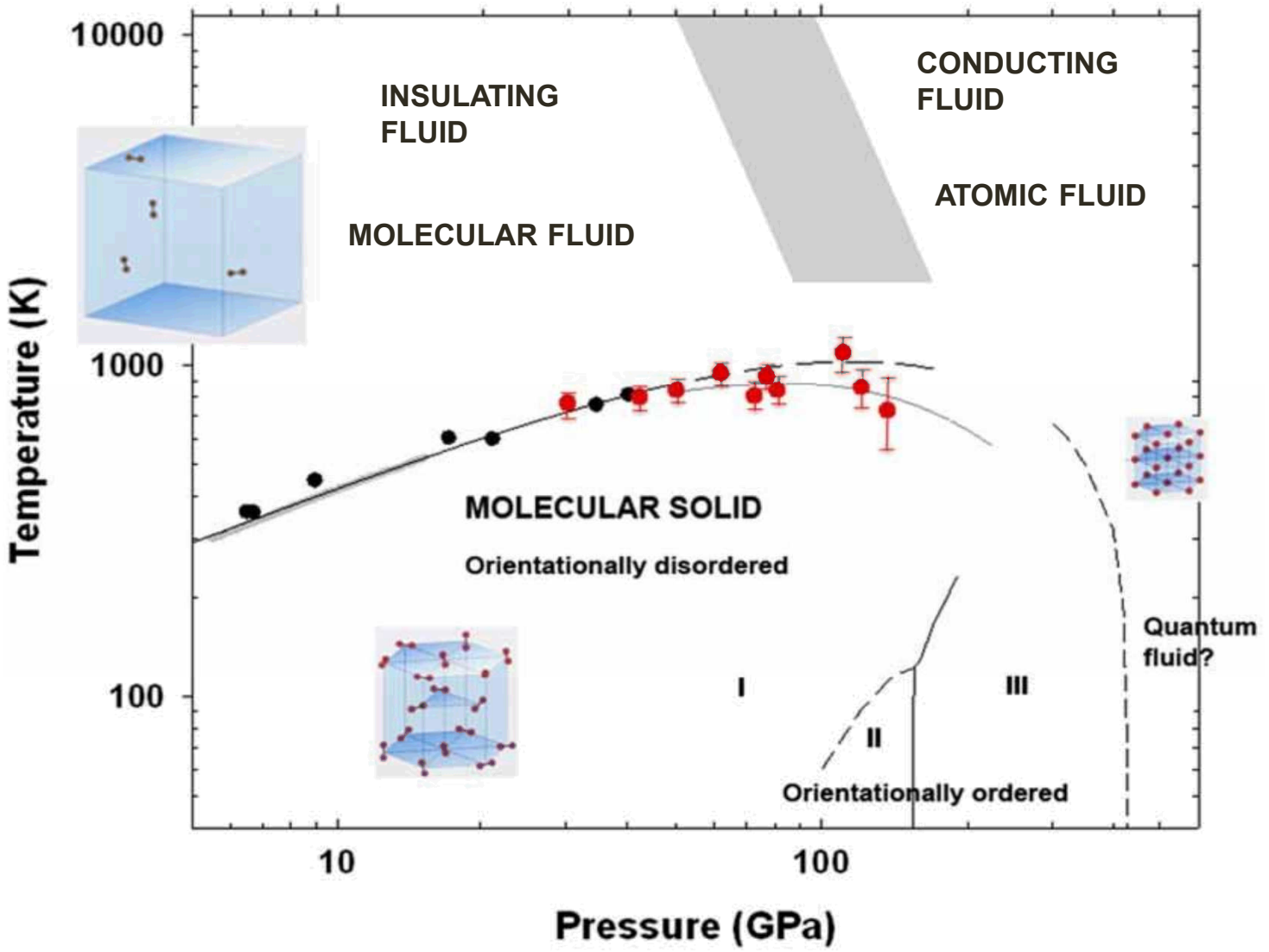
University of Rostock

Outline

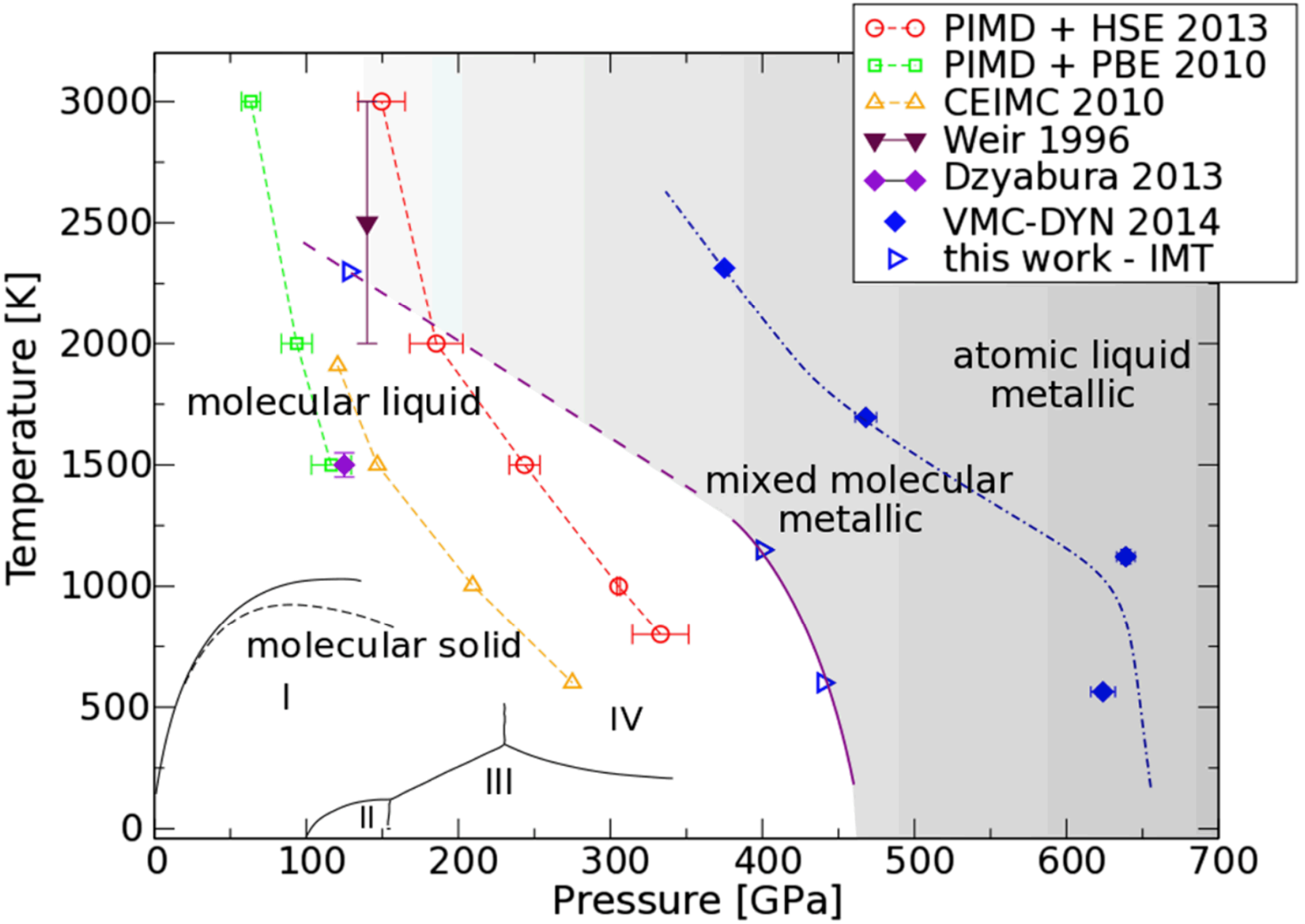
- liquid-liquid, insulator-to-metal transition (LL-IMT) in deuterium
  - Observed to be density driven and relatively insensitive to temperature
- low-density IMT along the Hugoniot in deuterium
  - Recent results show nearly an order-of-magnitude improvement in precision

Part of a Jovian Science Z Fundamental Science Project

Hydrogen at high pressures – the known phase diagram so far

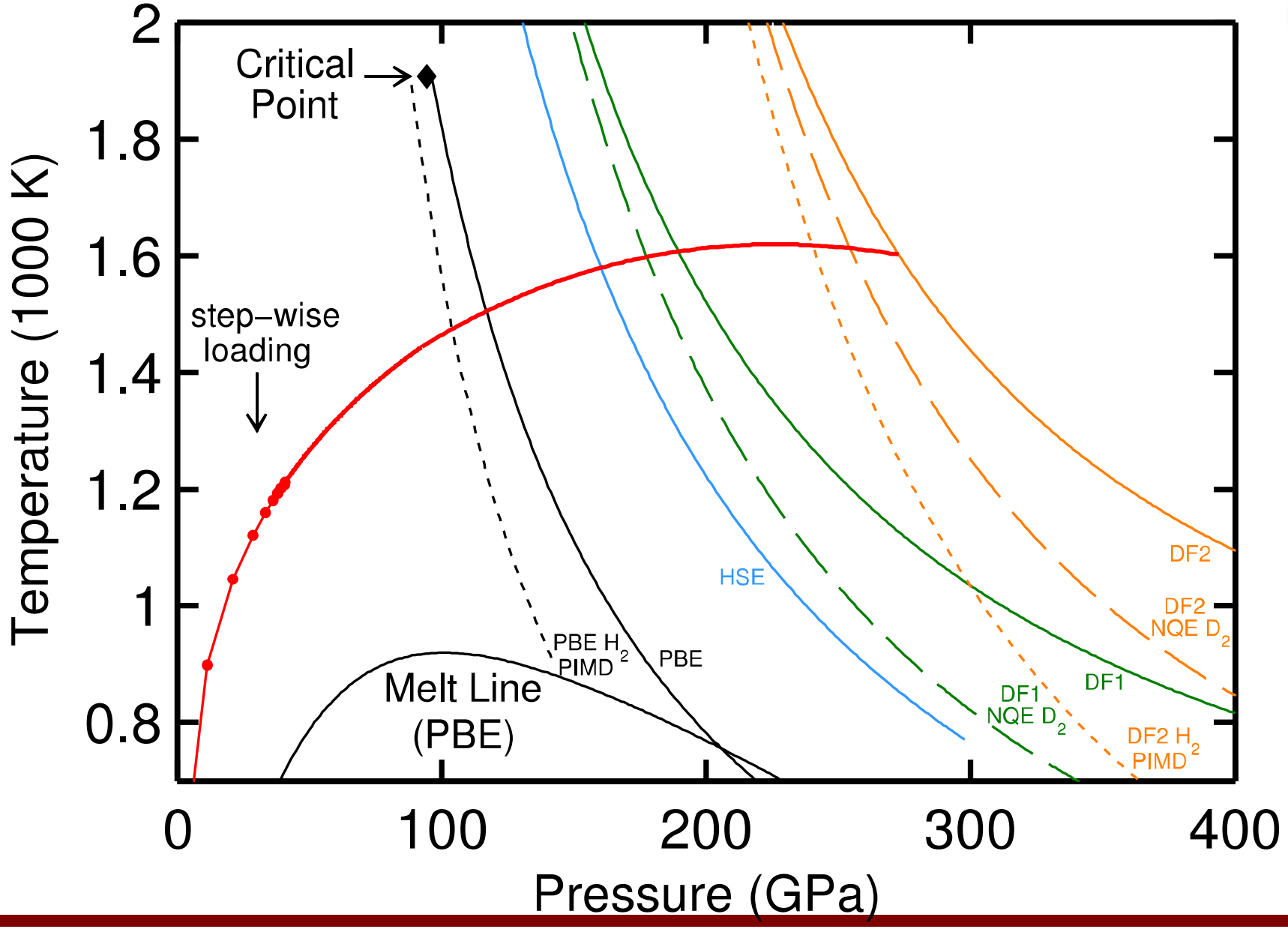


Recent predictions of the LL-IMT in hydrogen

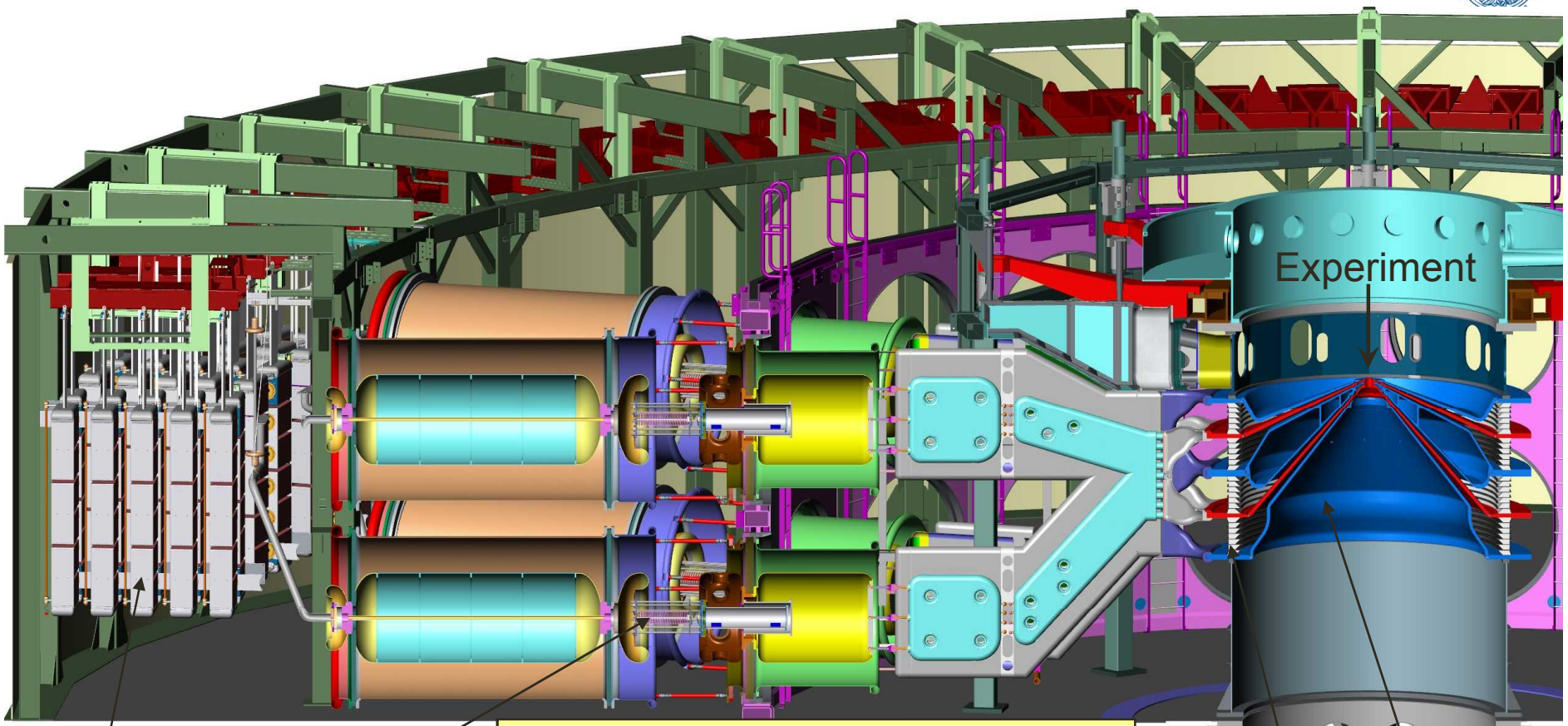


W. Lorenzen et al., PRB 82, 195107 (2010); PRB 84, 235109 (2011); PRL 107, 026401 (2011); PRB 89, 035109 (2014)

Proposed Experiment: Shock - Ramp



Sandia Z Machine



Marx generator

laser-triggered gas switch

22 MJ stored energy

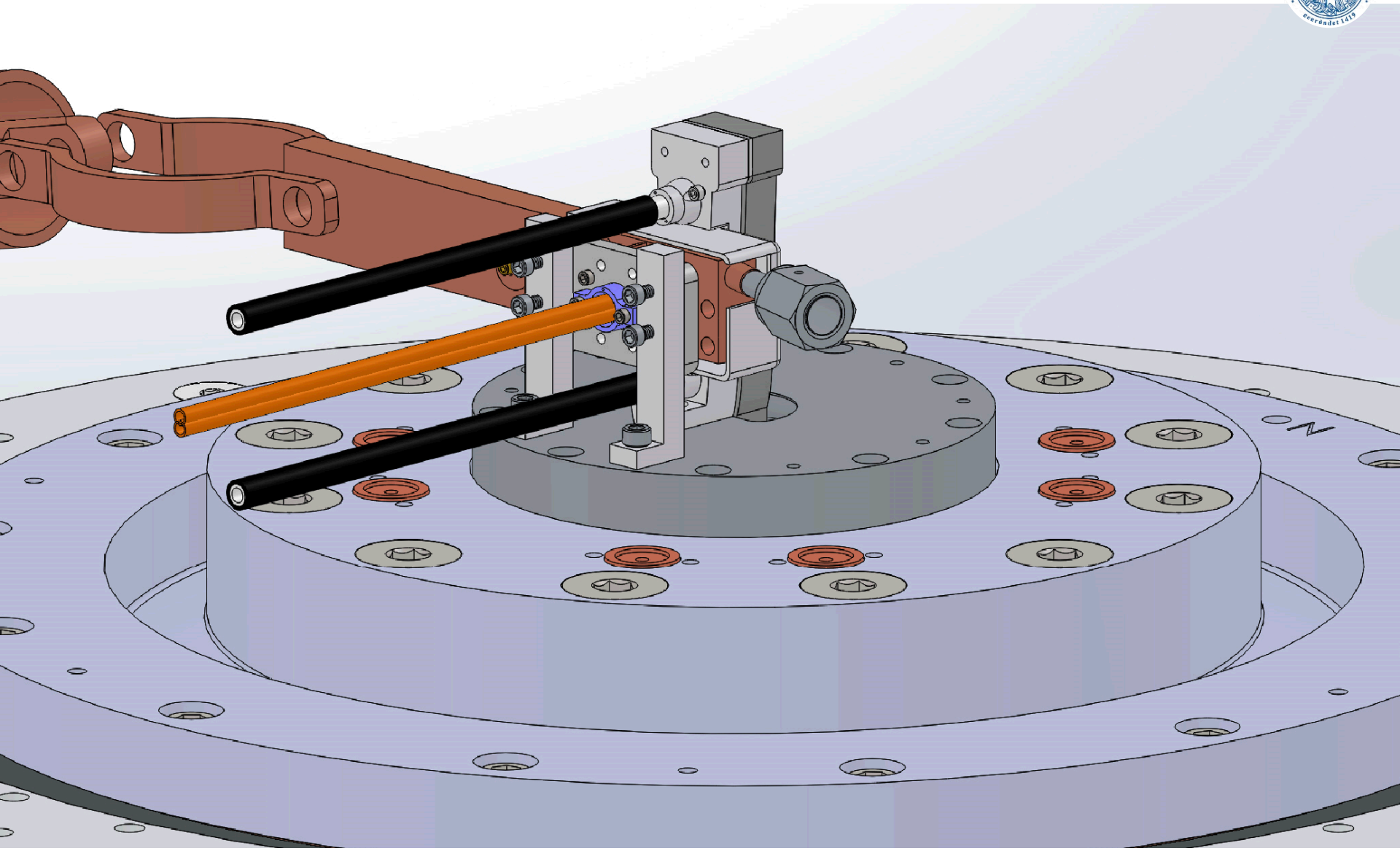
~25 MA peak current

~200-600 ns rise time

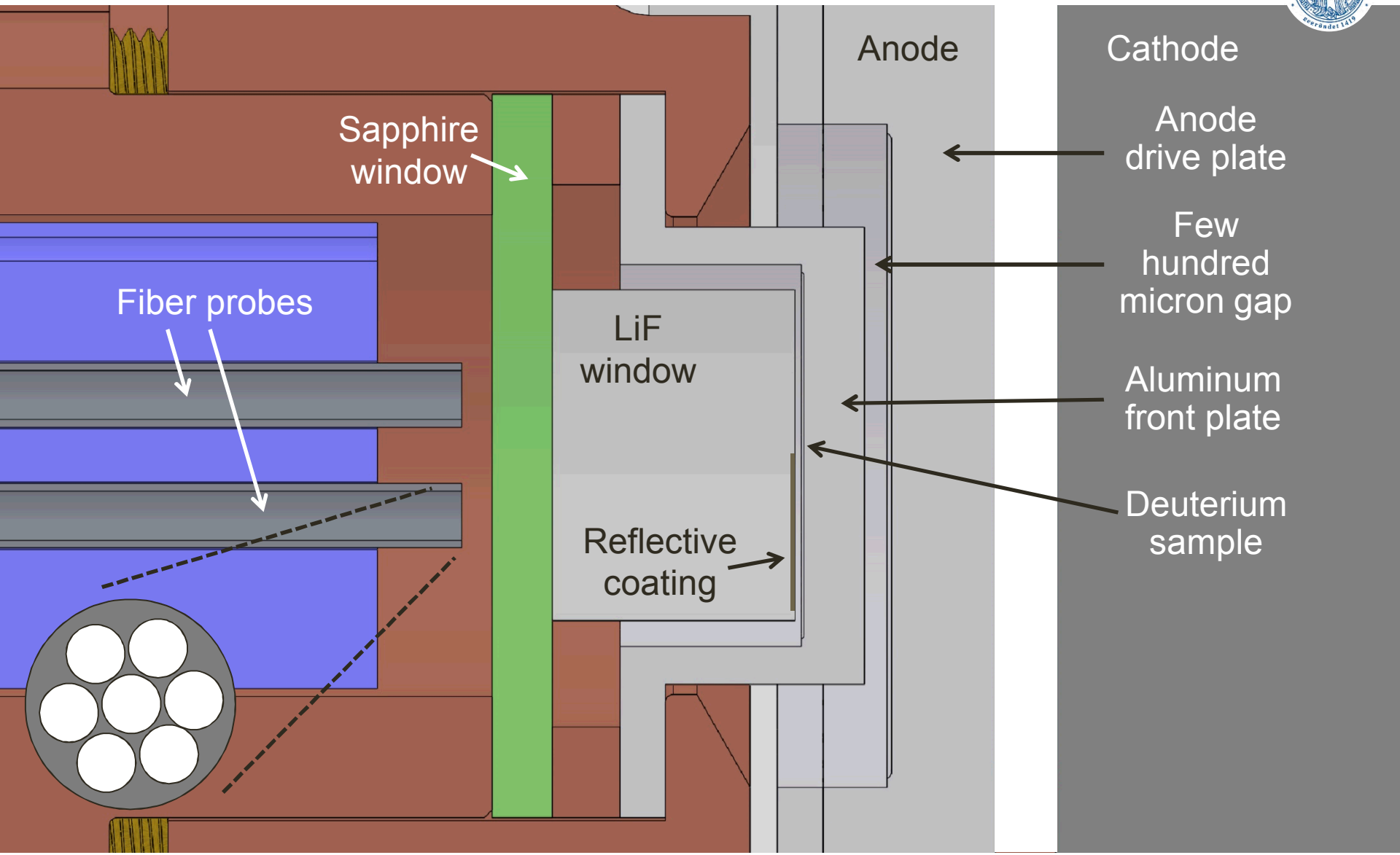
insulator stack

magnetically insulated transmission lines

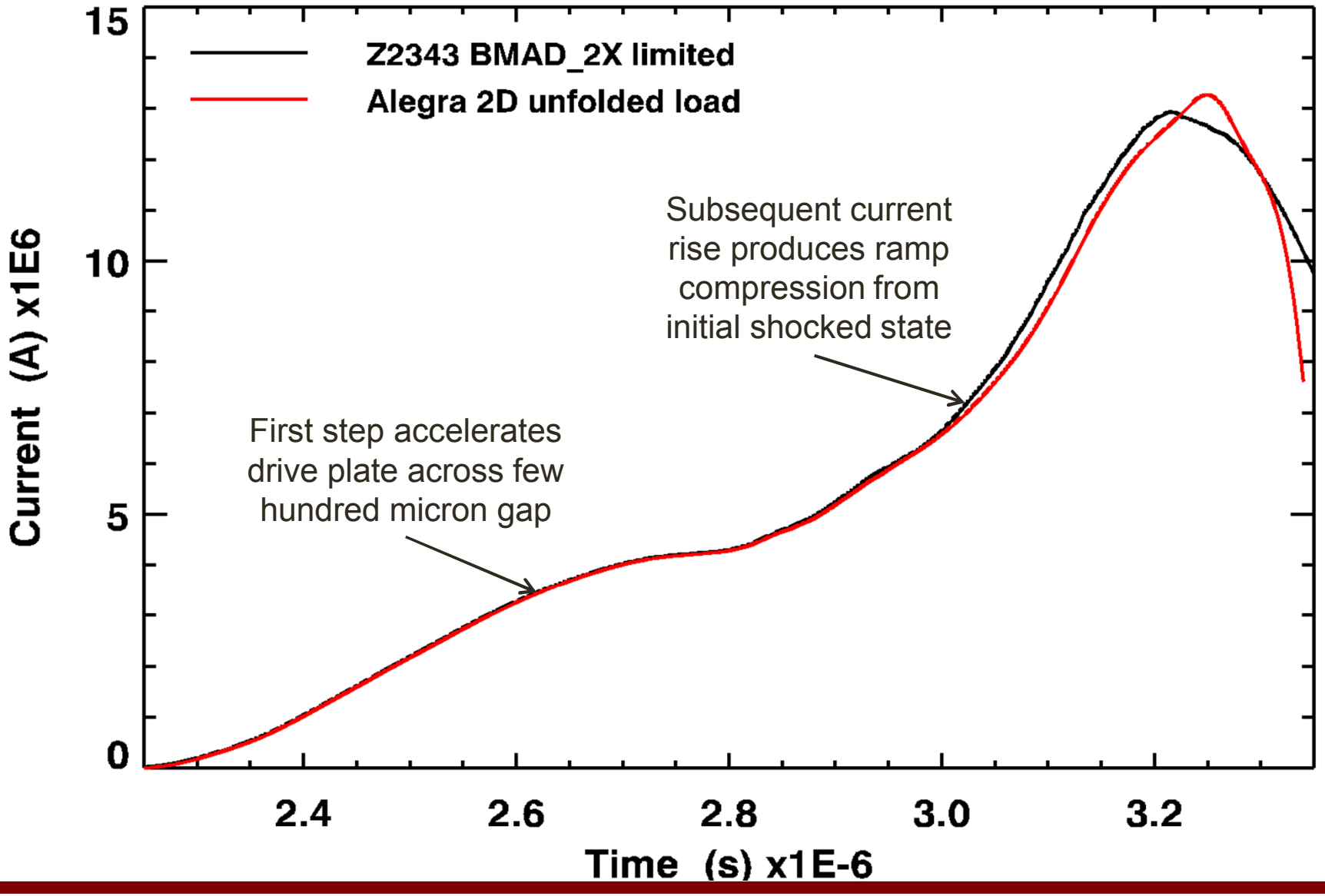
Experimental configuration



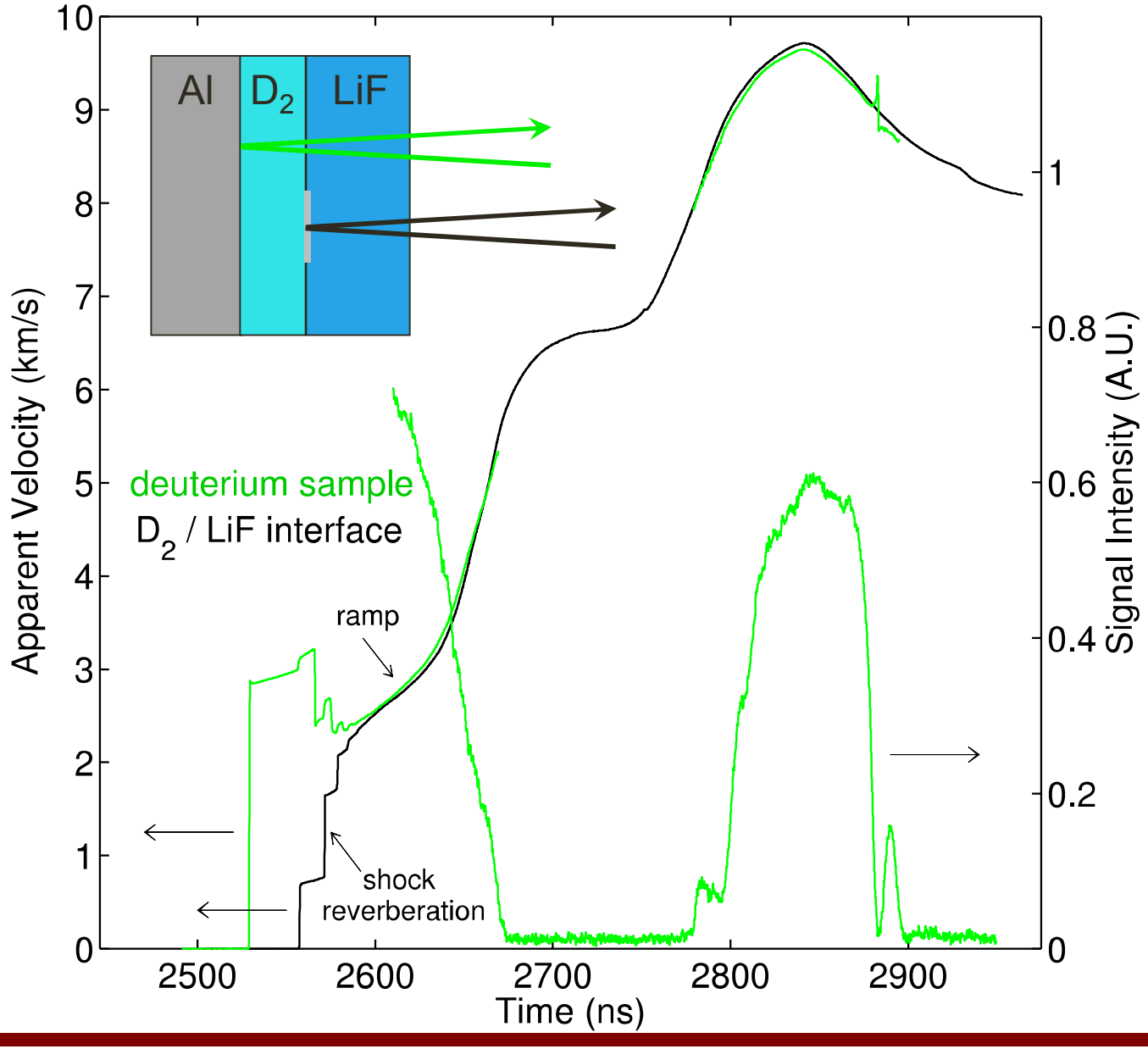
Experimental configuration



Two-step pulse shape provides shock-ramp profile



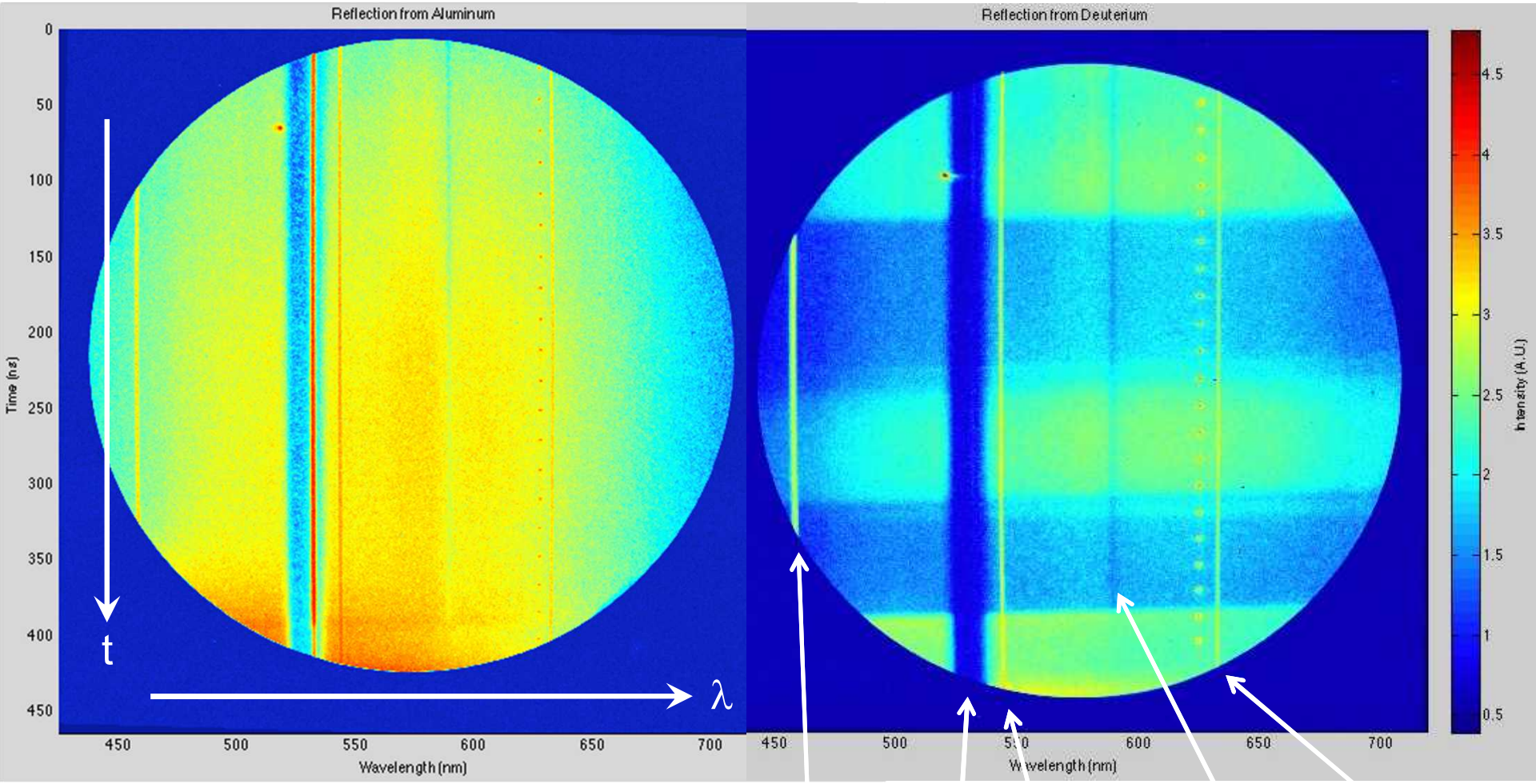
Measured observables in deuterium



SVS system provides data to infer reflectivity

Reflection from aluminum coating

Reflection from deuterium



Wavelength range ~450-700 nm

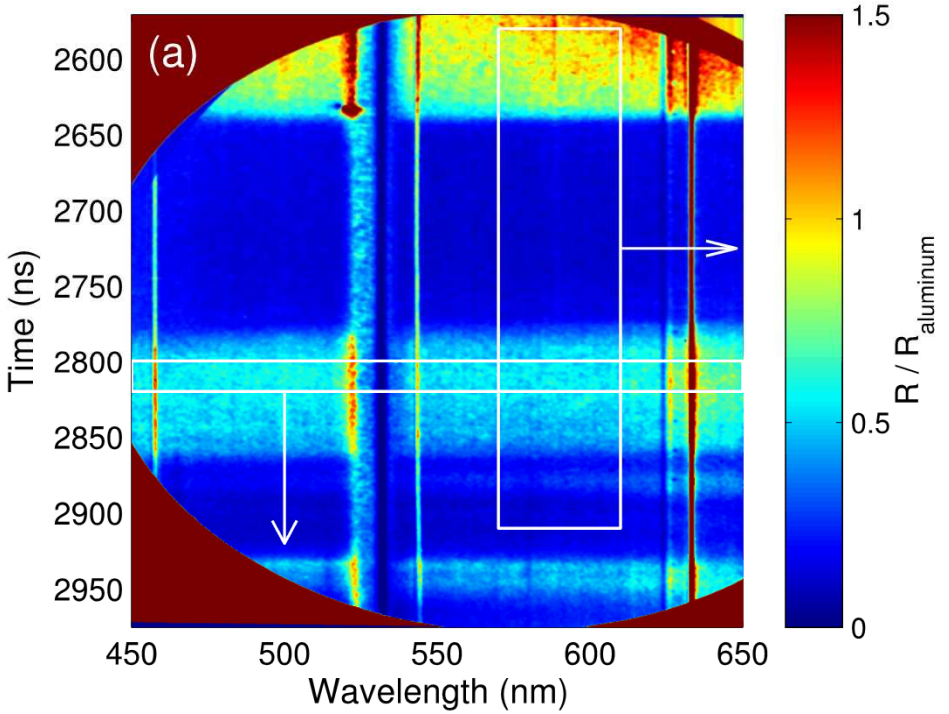
457.9 nm

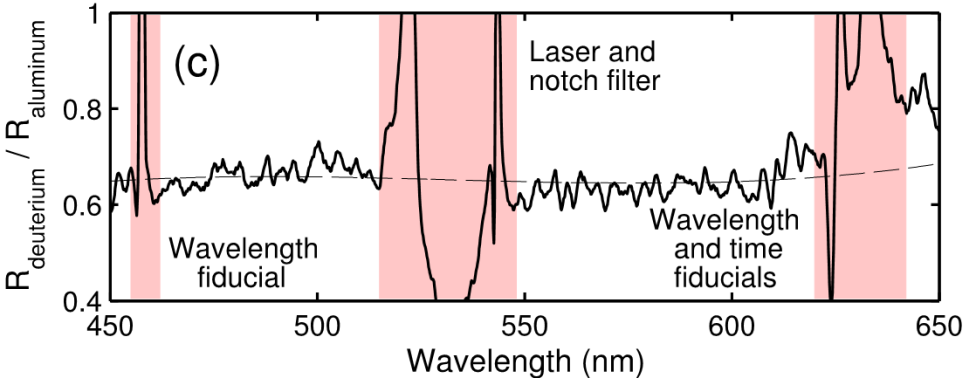
532 / 543.5 nm

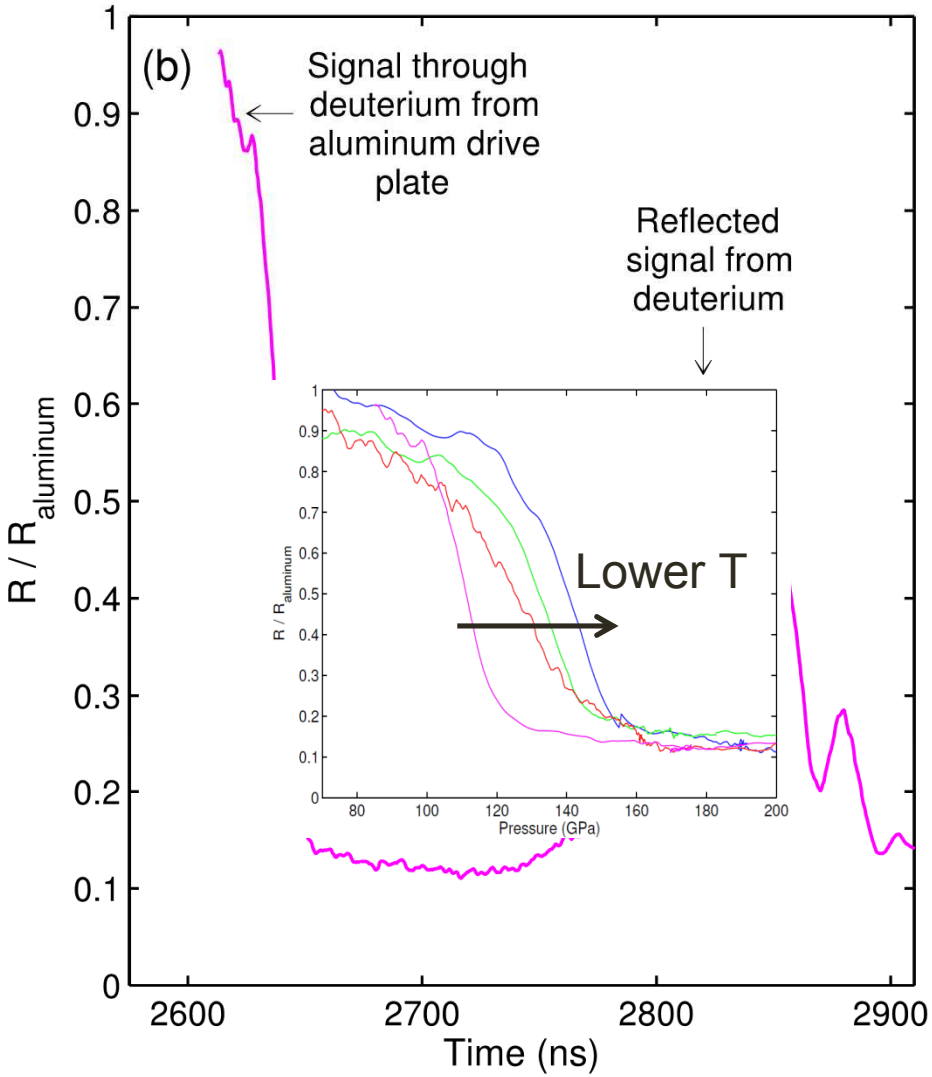
589.3 nm

633 nm

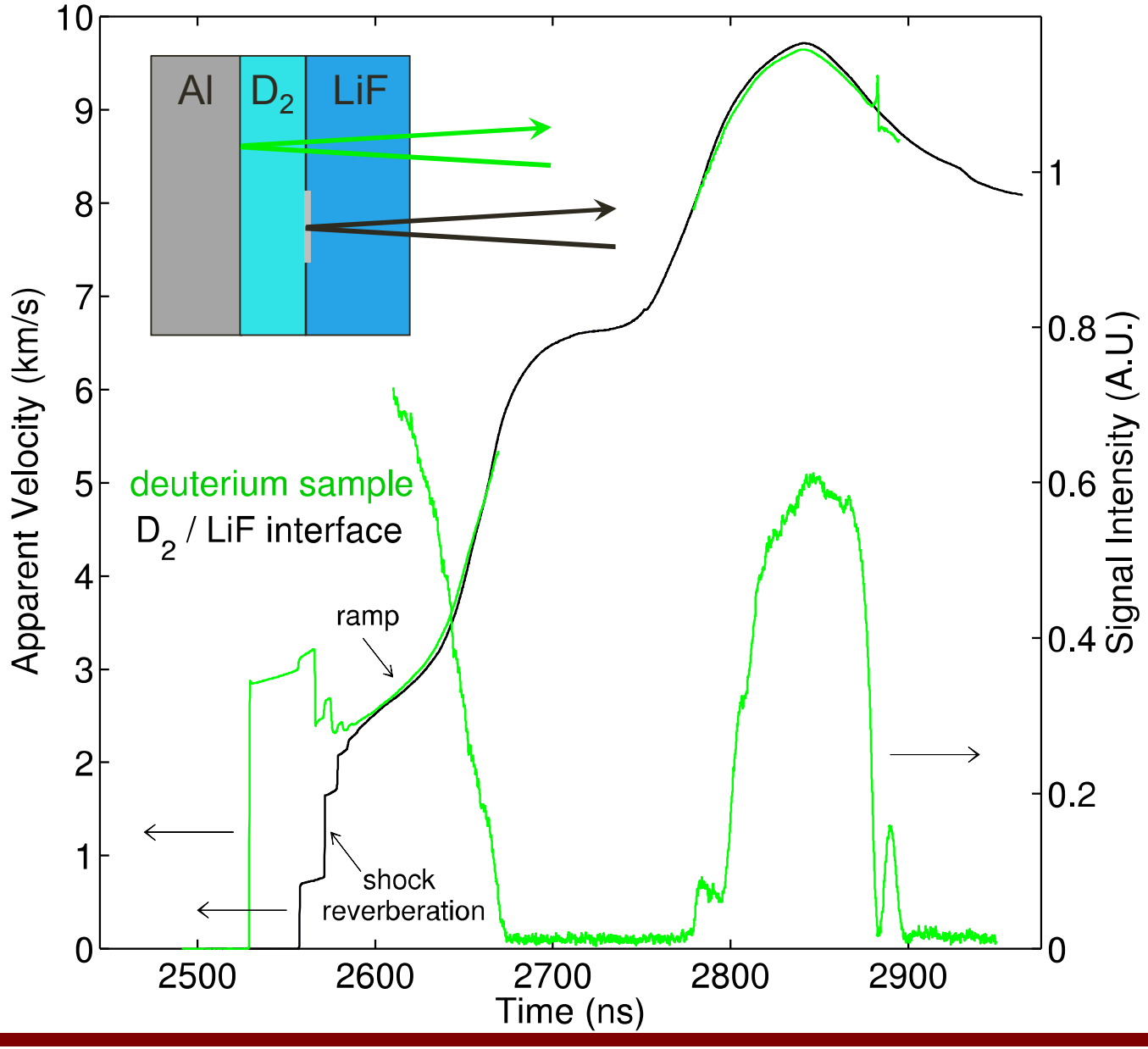
SVS system provides data to infer reflectivity



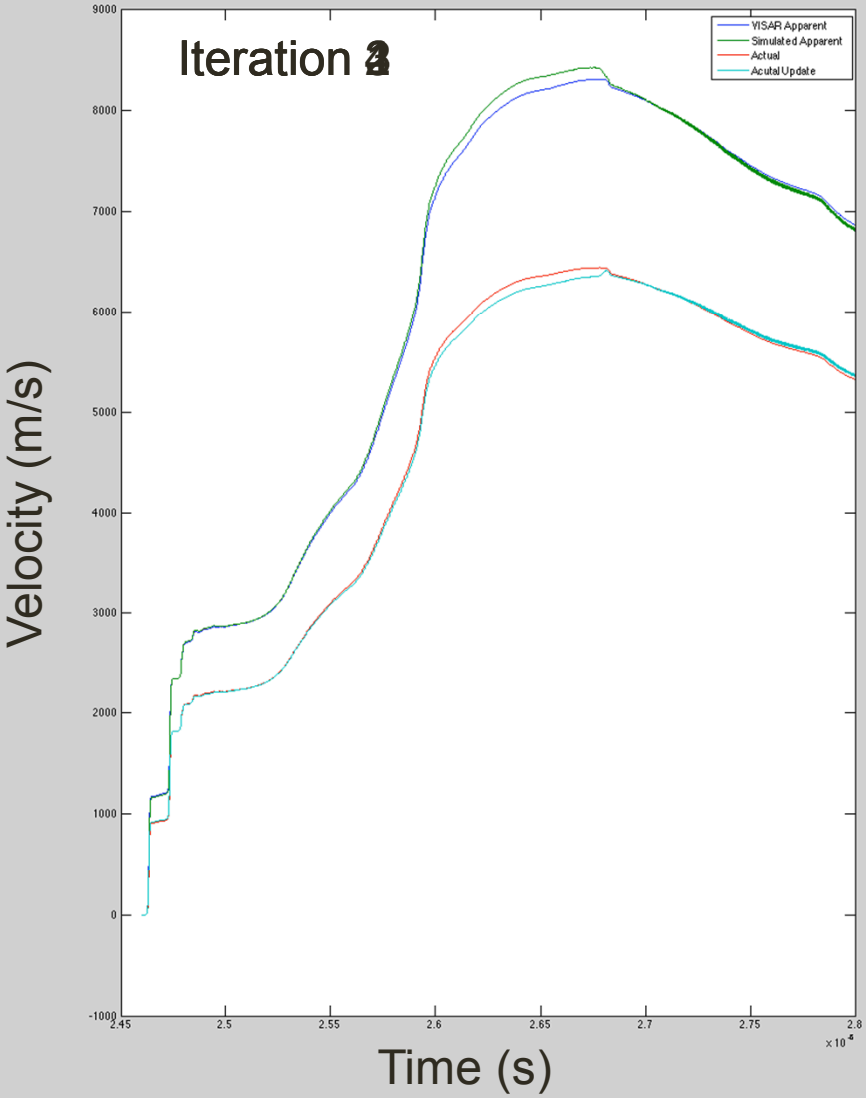


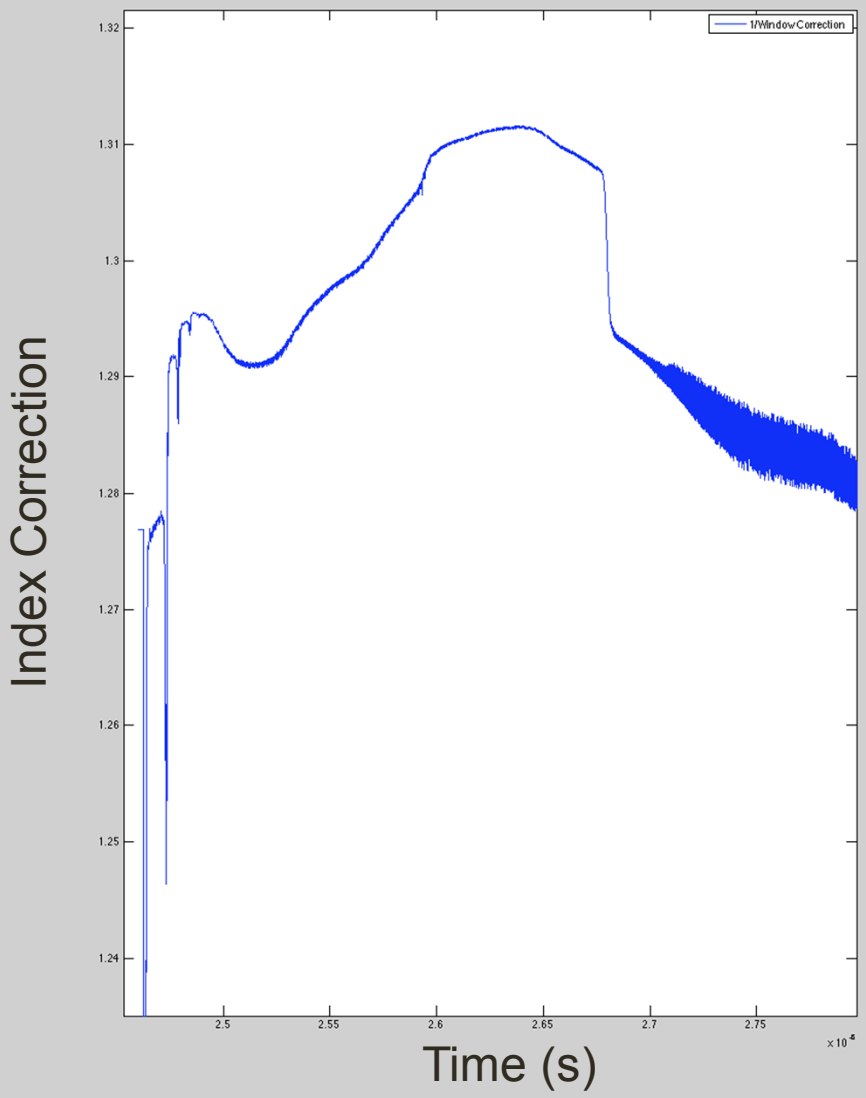


Measured observables in deuterium

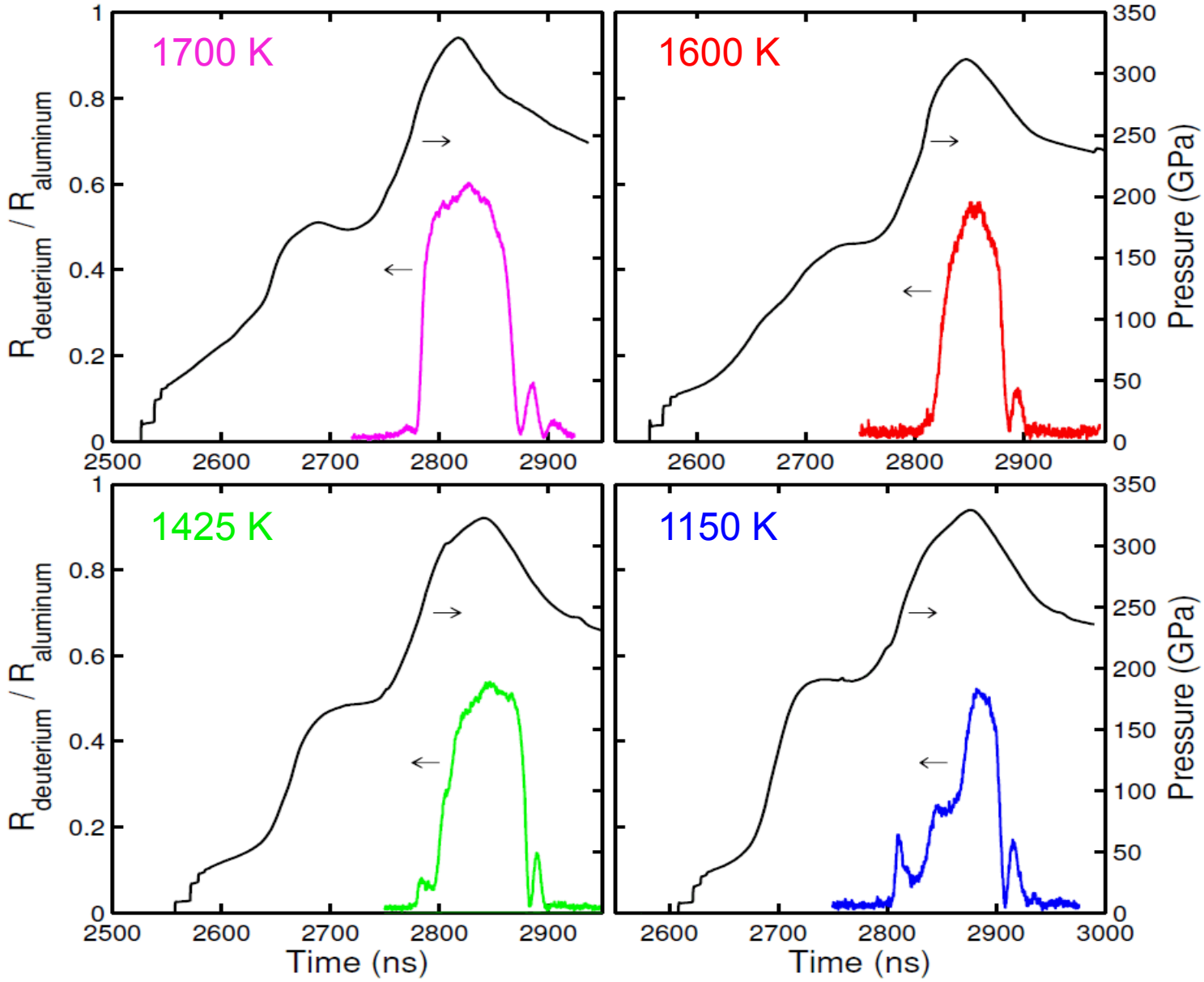


P(t) obtained from v(t) and LiF EOS

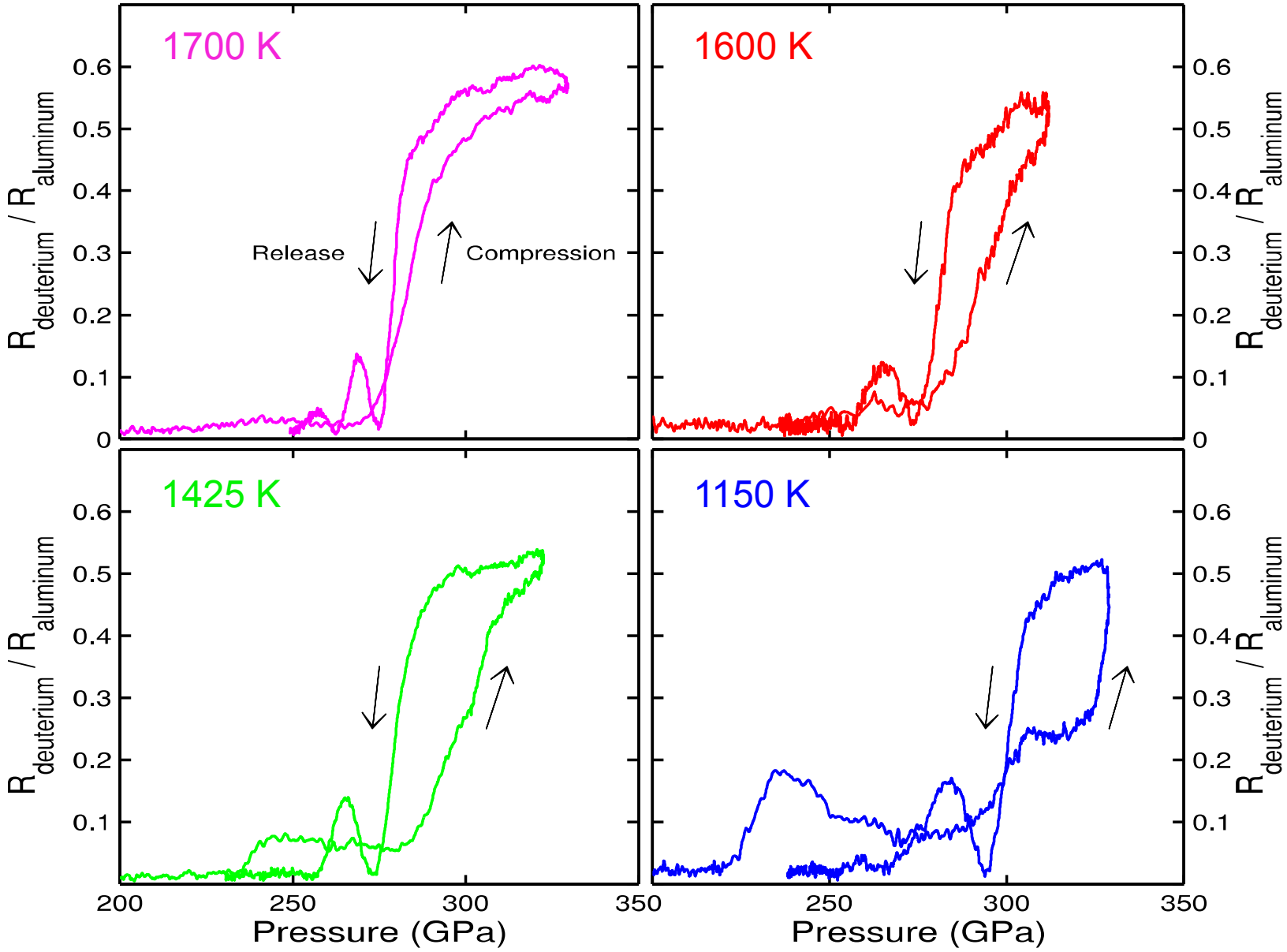




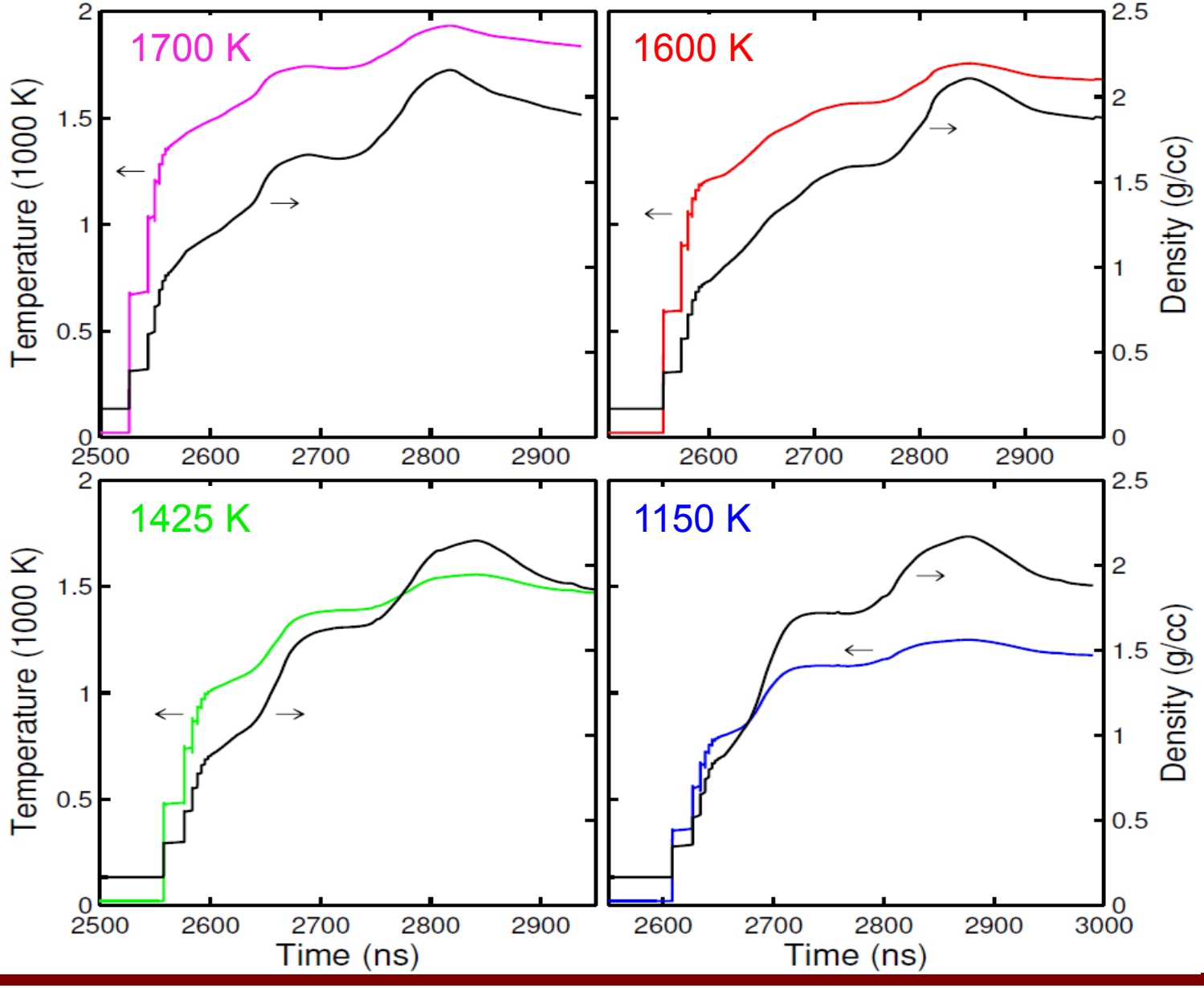
P(t) between ~1000-2000 K



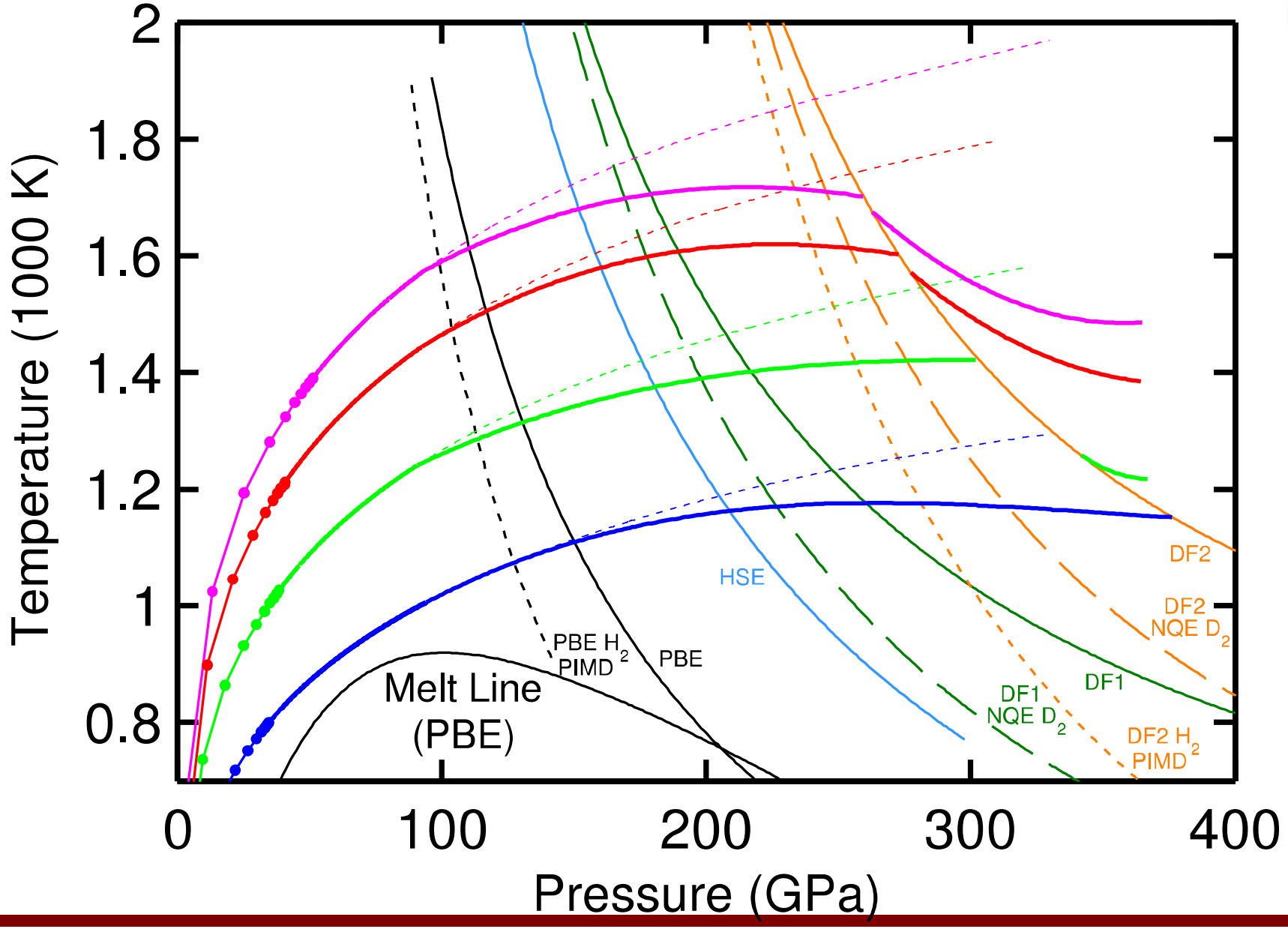
Reflectivity signals mapped to pressure



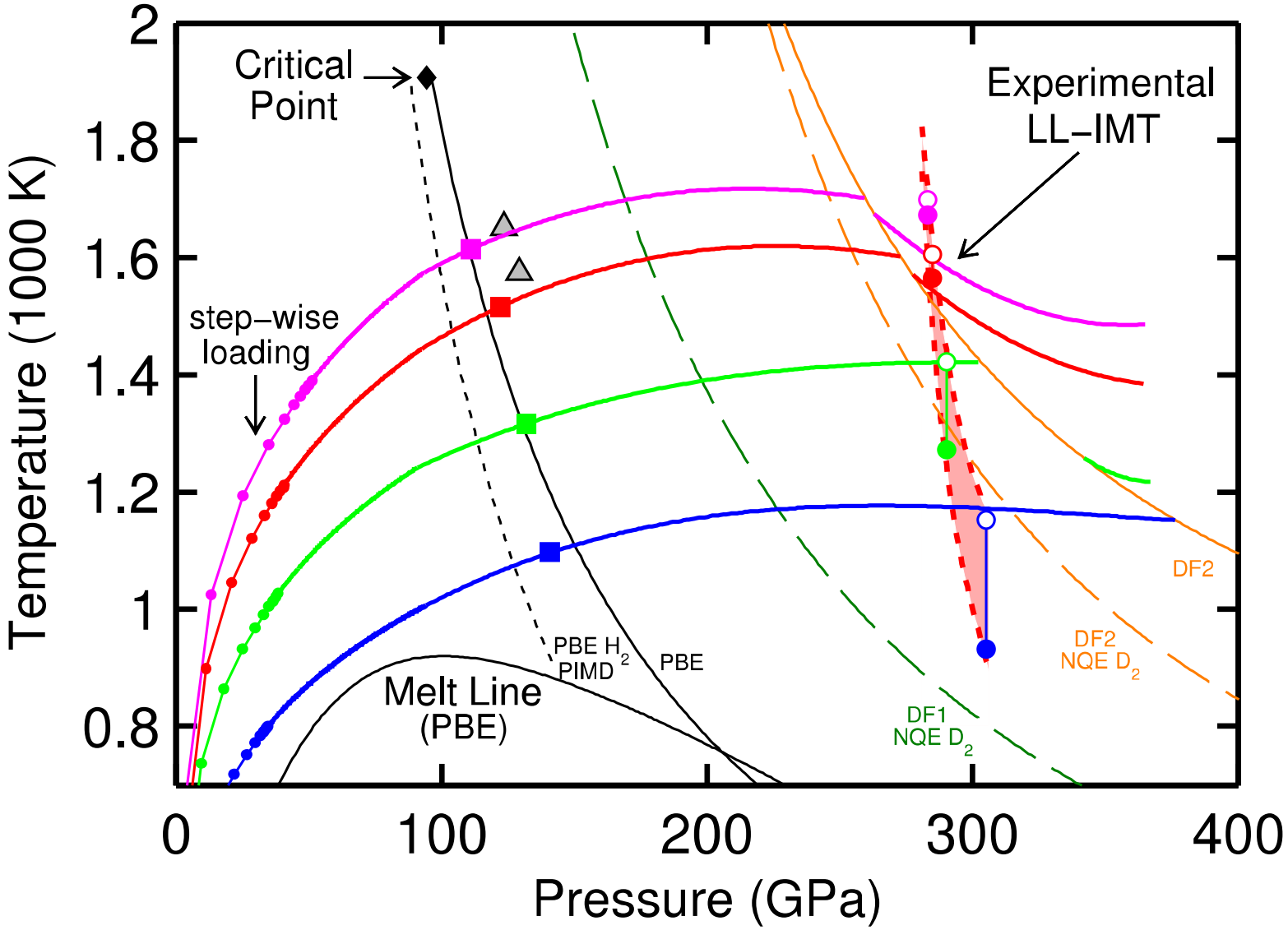
T(t) and ρ(t) obtained from D_2 EOS (Kerley03)



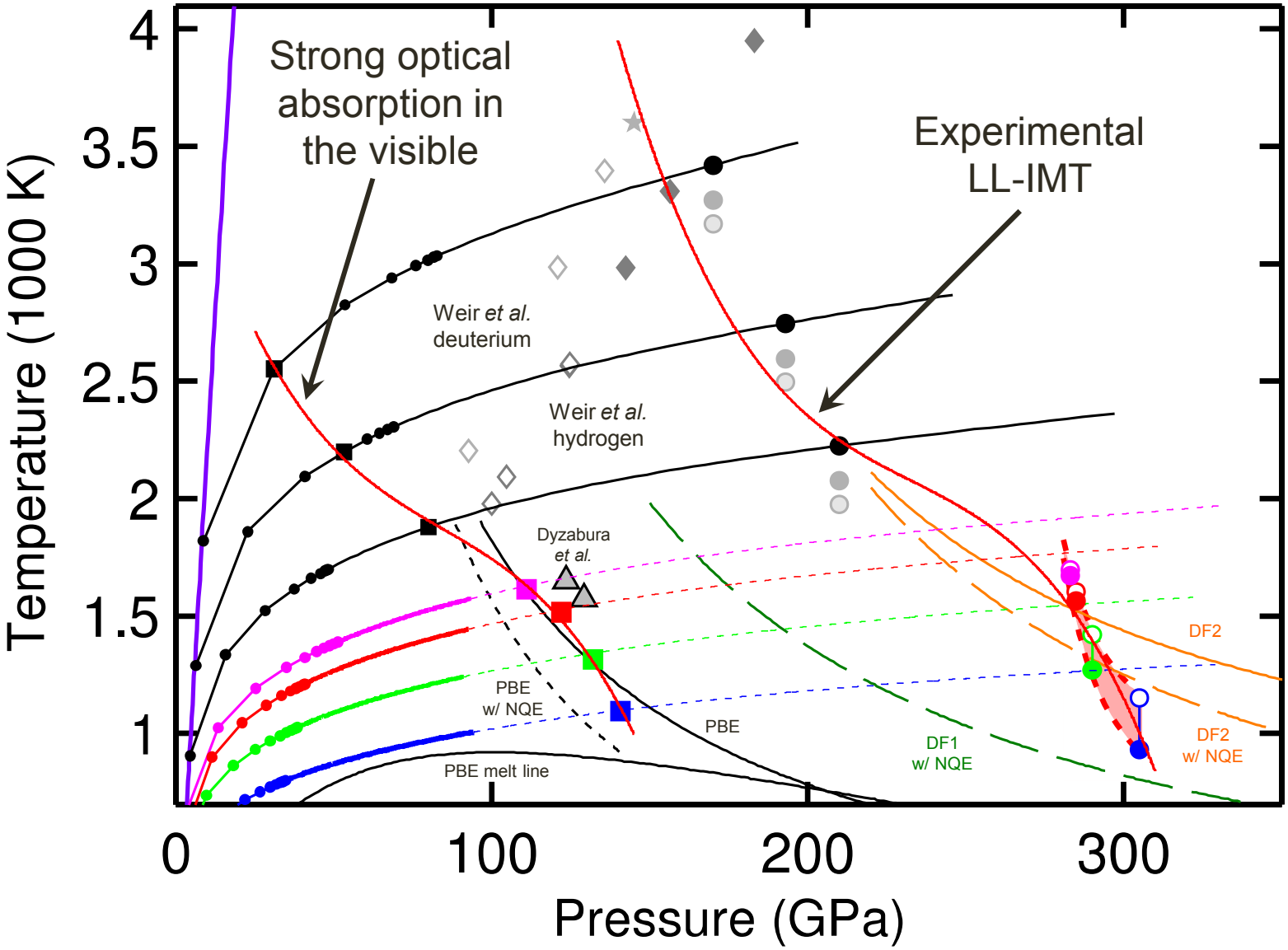
Experimental PT Paths



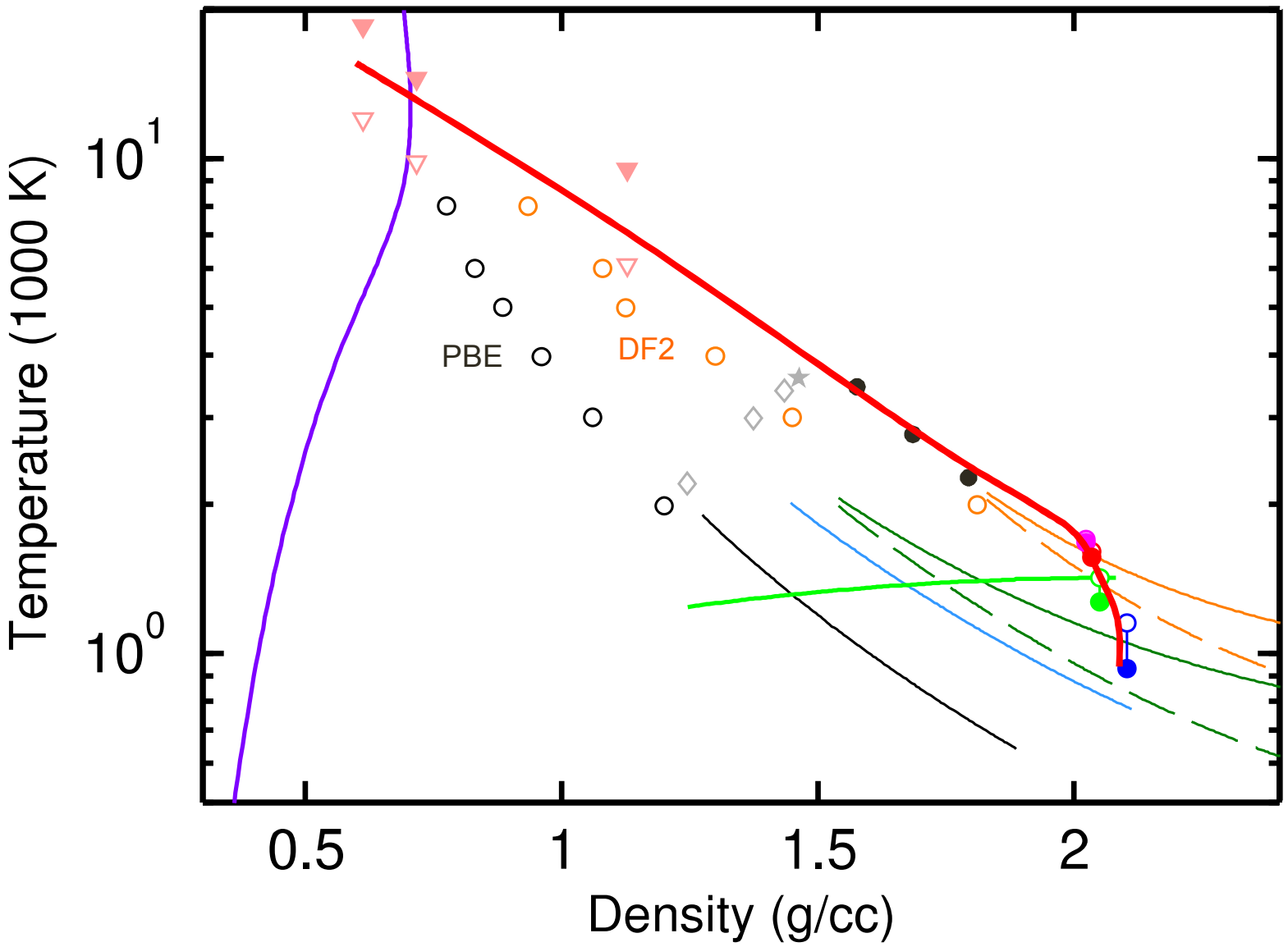
Location of the LL-IMT in deuterium



Location of the LL-IMT in deuterium



Extended P-ρ diagram for deuterium

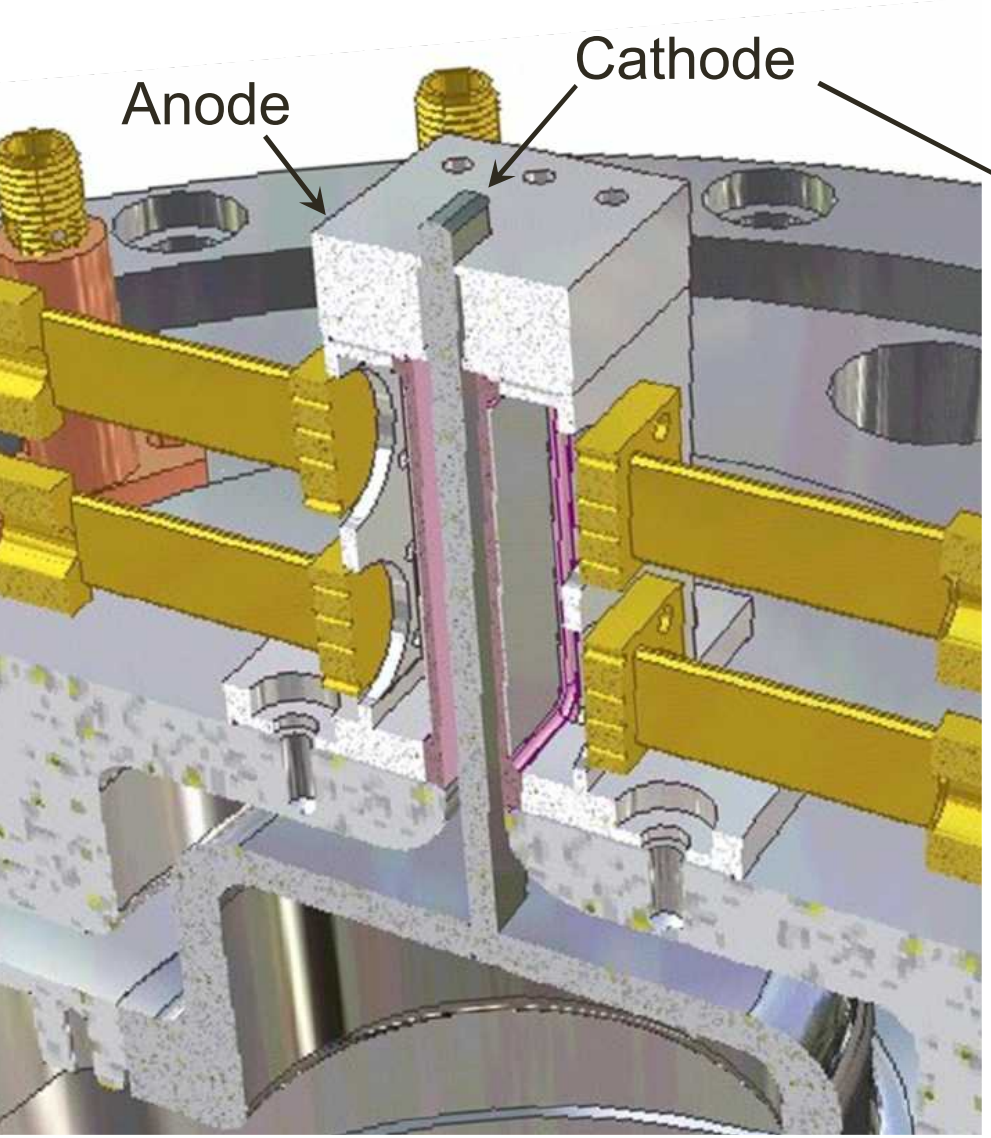


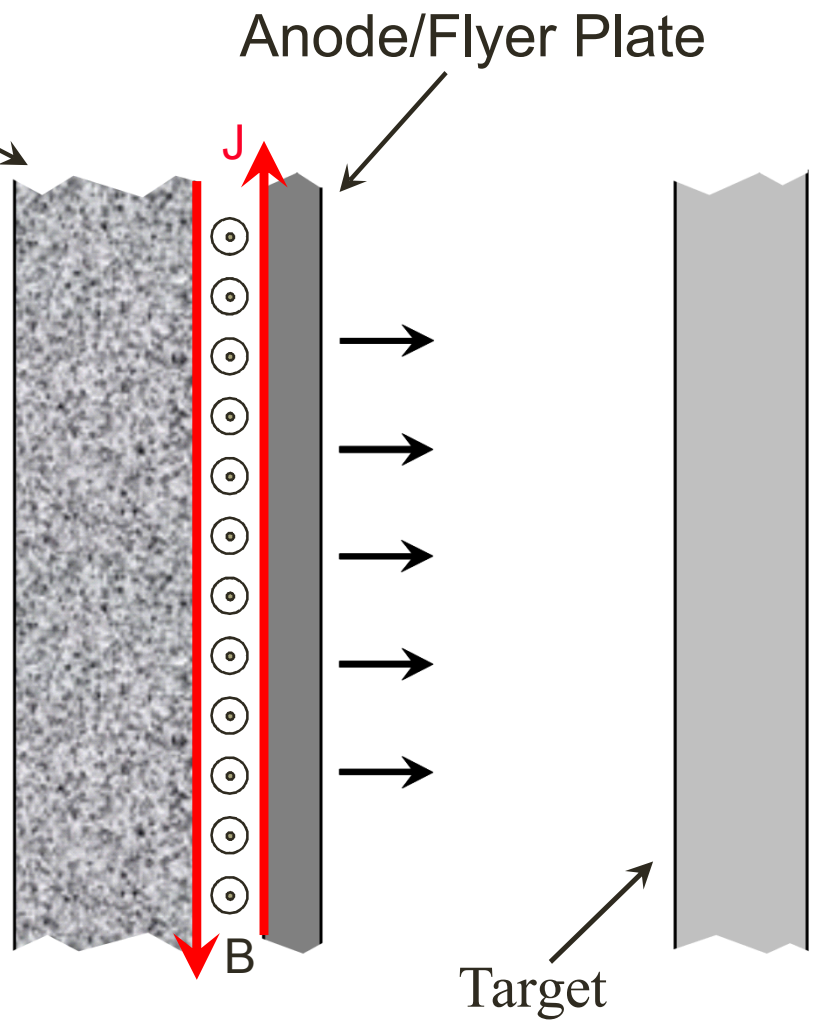
Outline

- liquid-liquid, insulator-to-metal transition (LL-IMT) in deuterium
  - Observed to be density driven and relatively insensitive to temperature
- low-density IMT along the Hugoniot in deuterium
  - Recent results show nearly an order-of-magnitude improvement in precision

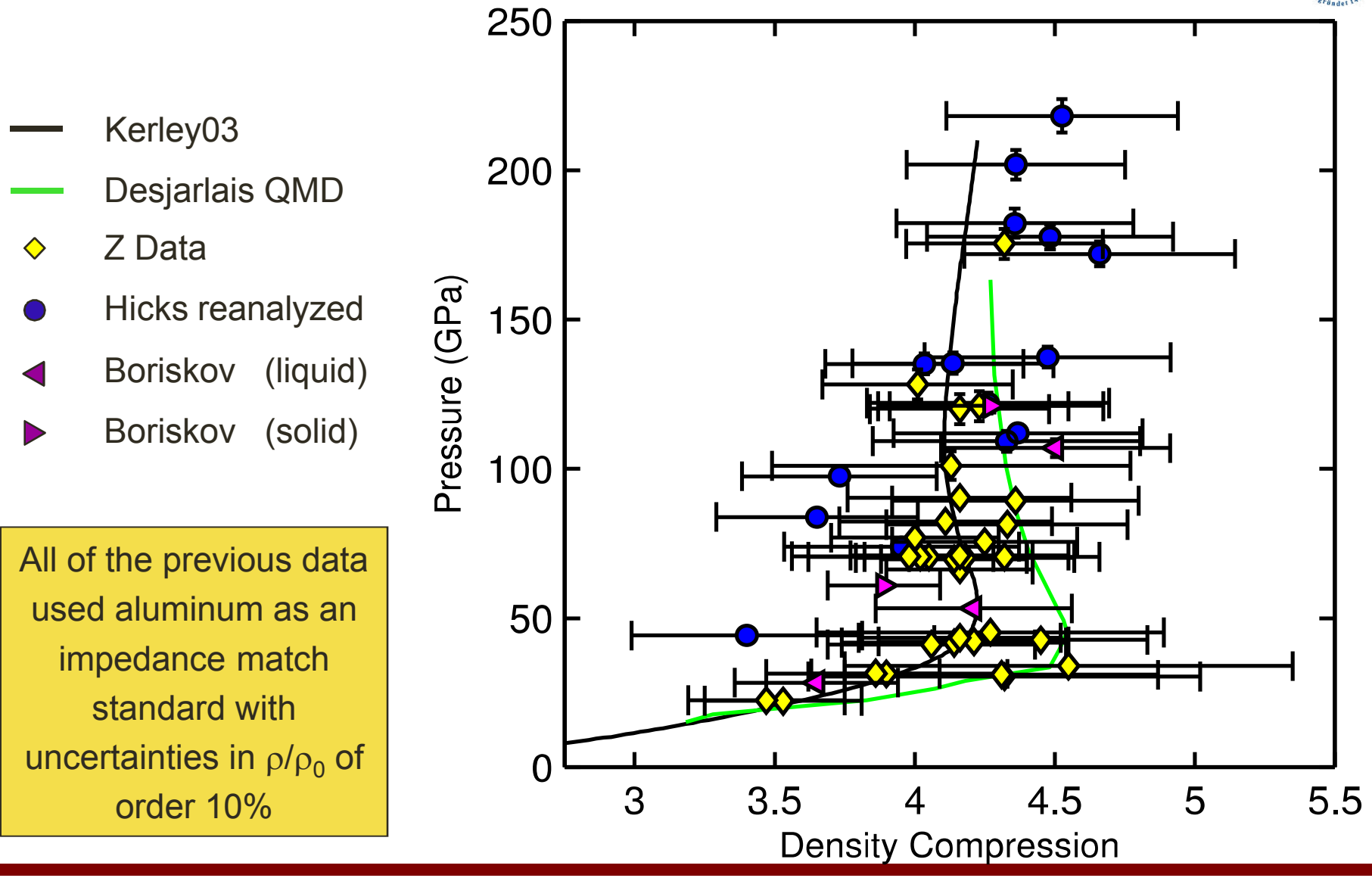
Part of a Jovian Science Z Fundamental Science Project

Magnetic pressure can also be used to launch flyer plates to high velocity





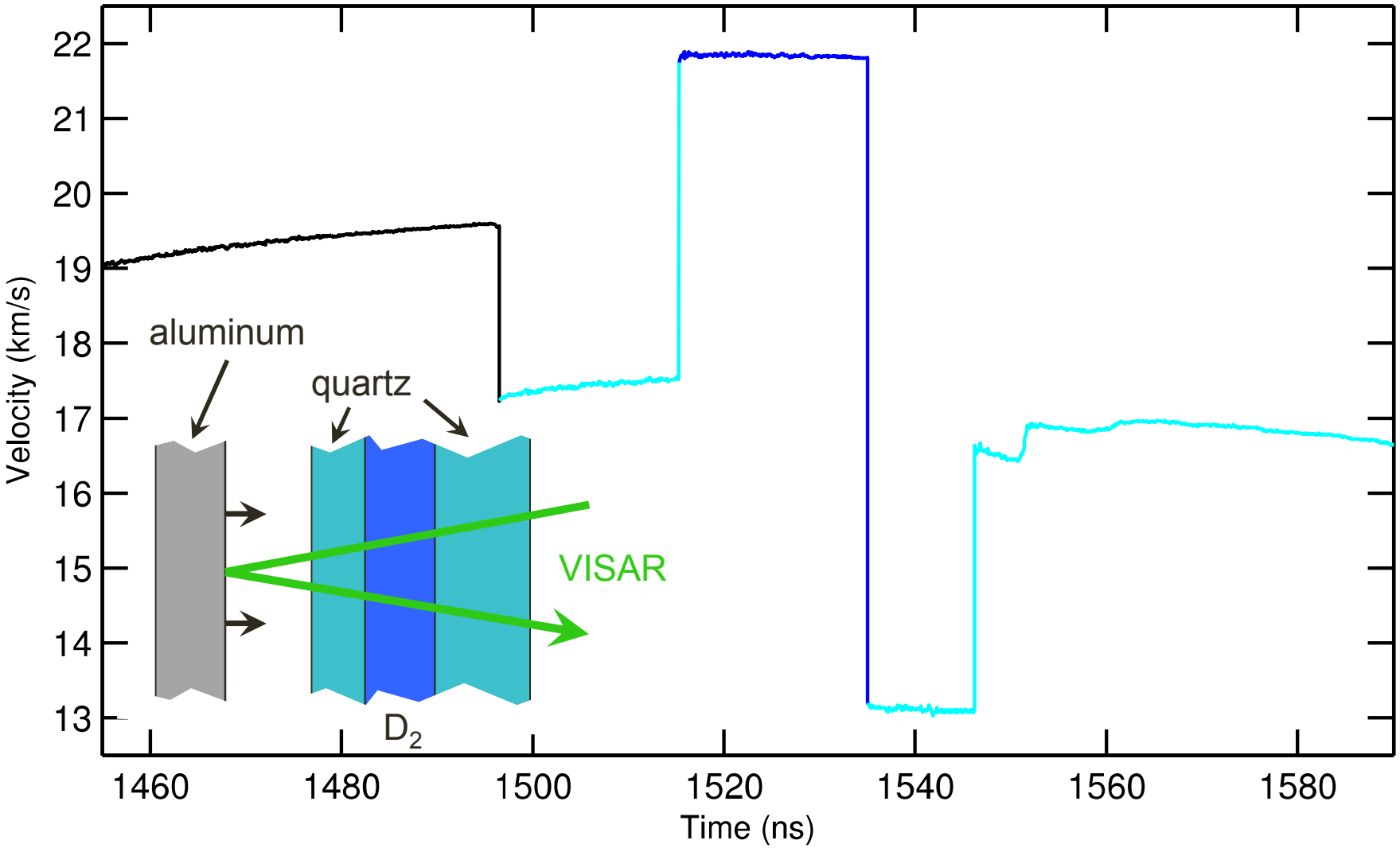
Previous Hugoniot data for deuterium has relatively large uncertainty and scatter



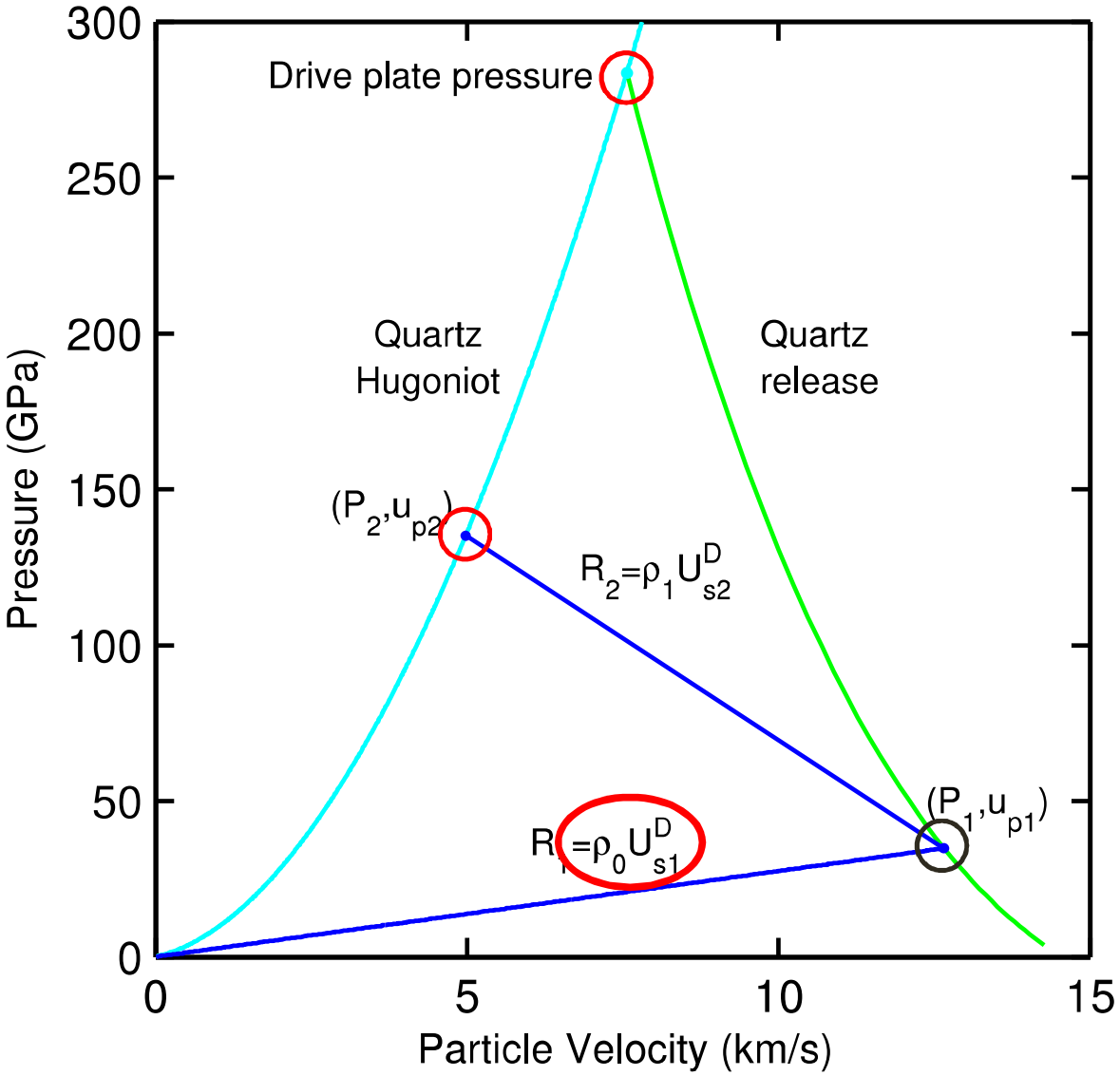
All of the previous data used aluminum as an impedance match standard with uncertainties in ρ/ρ_0 of order 10%

Boriskov et al., PRB 71, 092104 (2005) Knudson et al., PRB 69, 144209 (2004) Hicks et al., PRB 79, 014112 (2009)

VISAR was used to obtain precise flyer plate and shock velocities in the D_2 and quartz

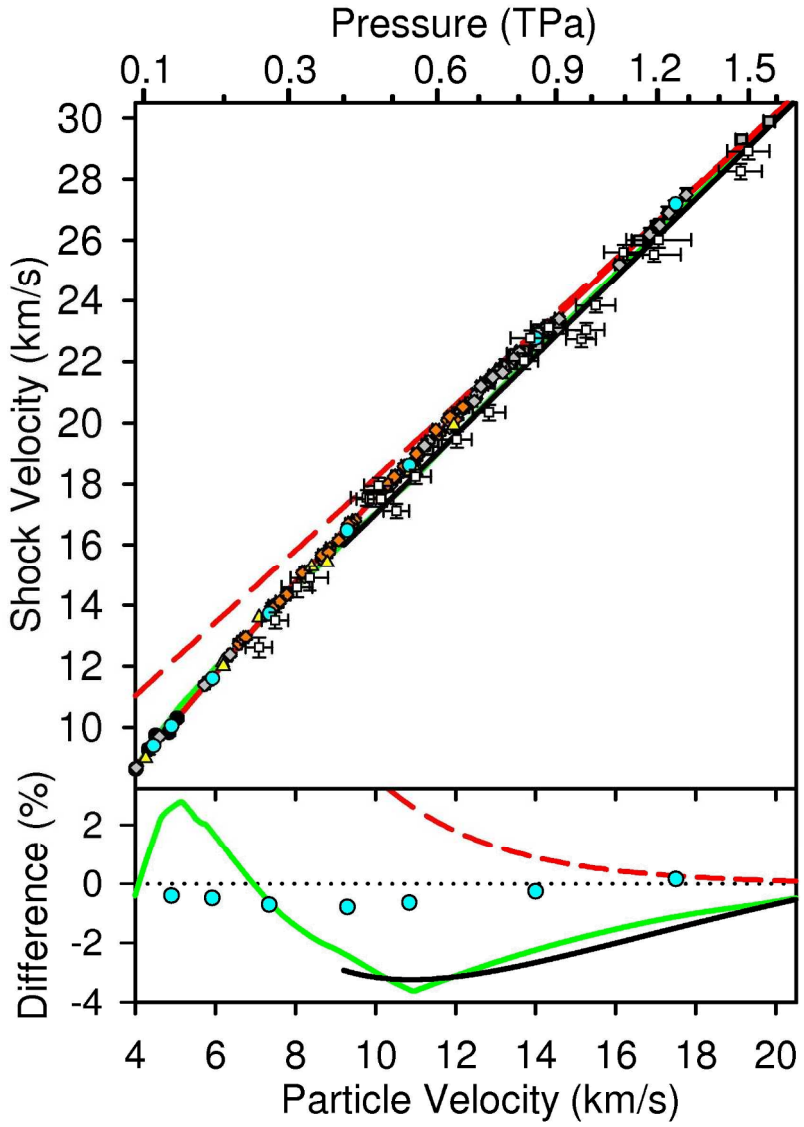


Shock response of D_2 is determined through impedance matching with quartz standard

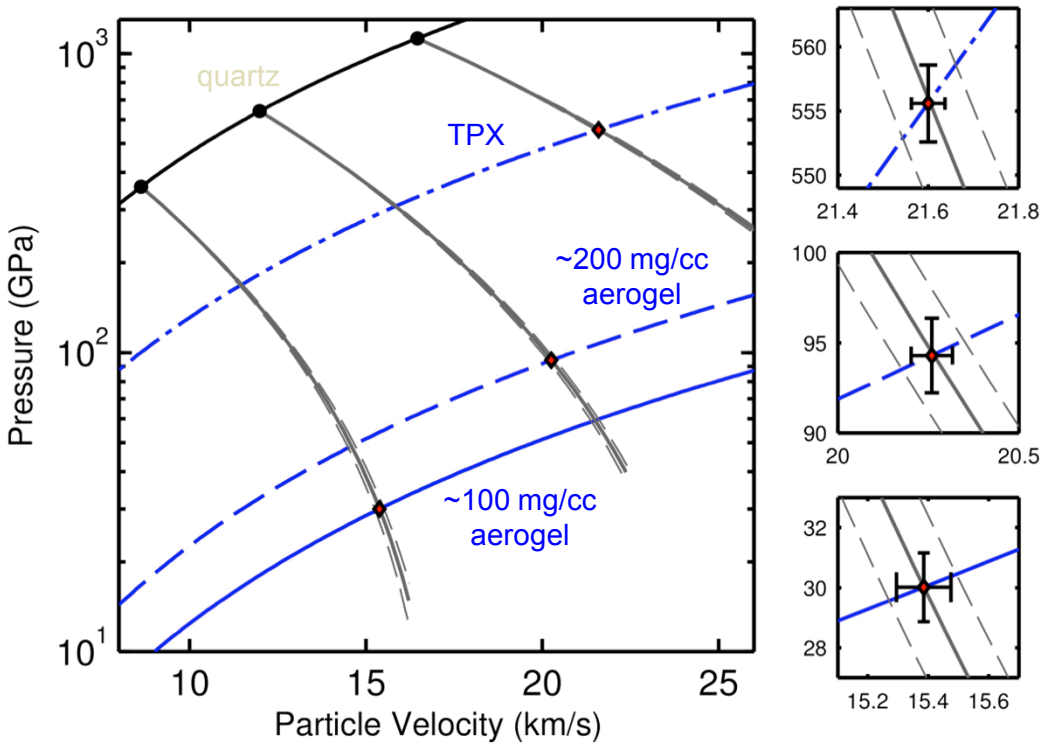


- Measured Us in quartz determines (P, u_p) for drive plate
- The empirical release model is used to calculate the release adiabat
- Intersection of the release adiabat and first shock Rayleigh line determines (P_1, u_{p1}) for deuterium
- Measured Us in quartz rear plate determines (P_2, u_{p2}) in deuterium

Quartz Hugoniot and release has been extensively studied in the multi-Mbar regime



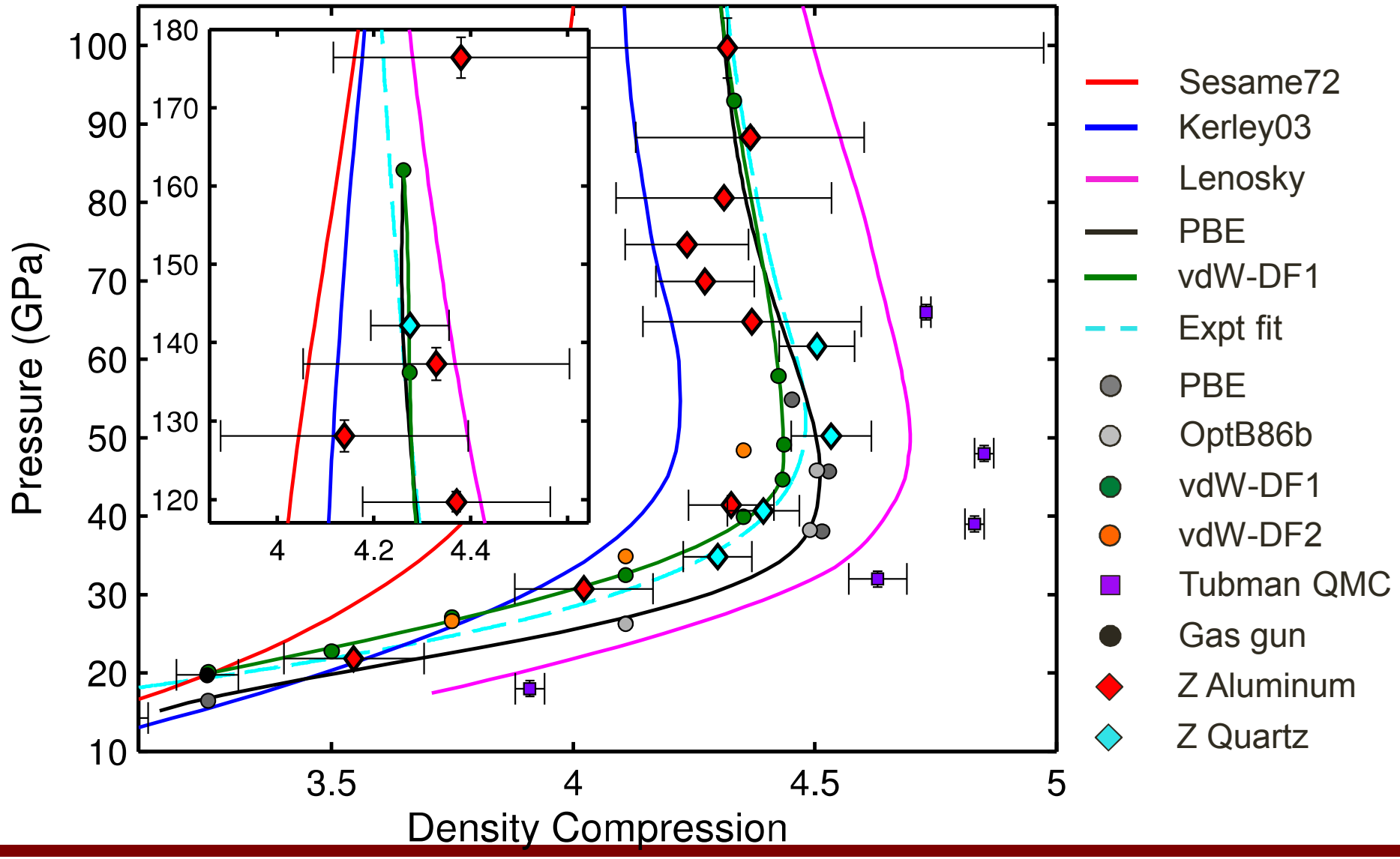
- Nearly 300 Hugoniot points for quartz have been obtained between 1 and 15 Mbar
- A release model was developed using release measurements obtained from TPX, and both ~200 mg/cc and ~100 mg/cc aerogel



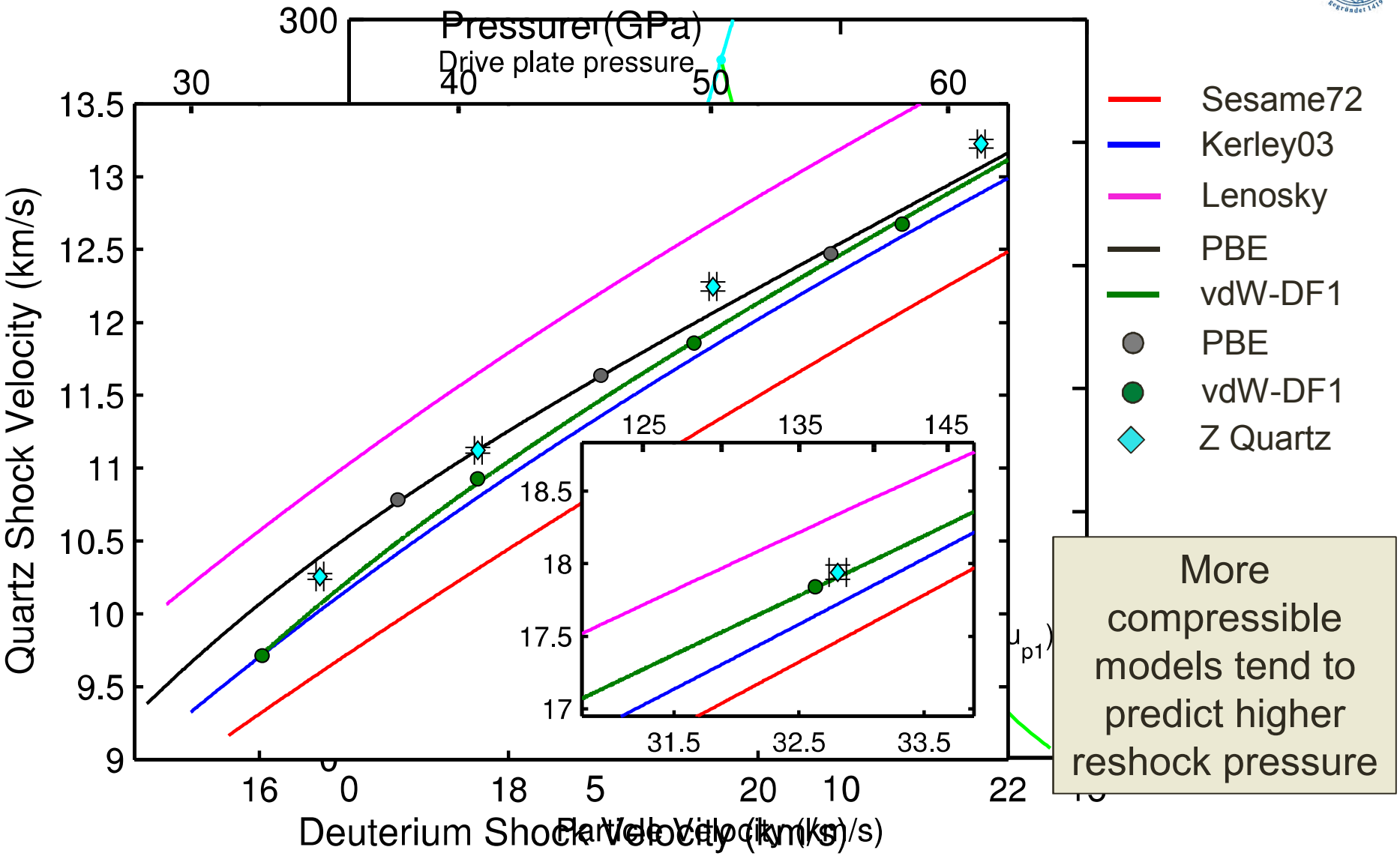
Knudson and Desjarlais, PRL 103, 225501 (2009)

Knudson and Desjarlais, PRB 88, 184107 (2013)

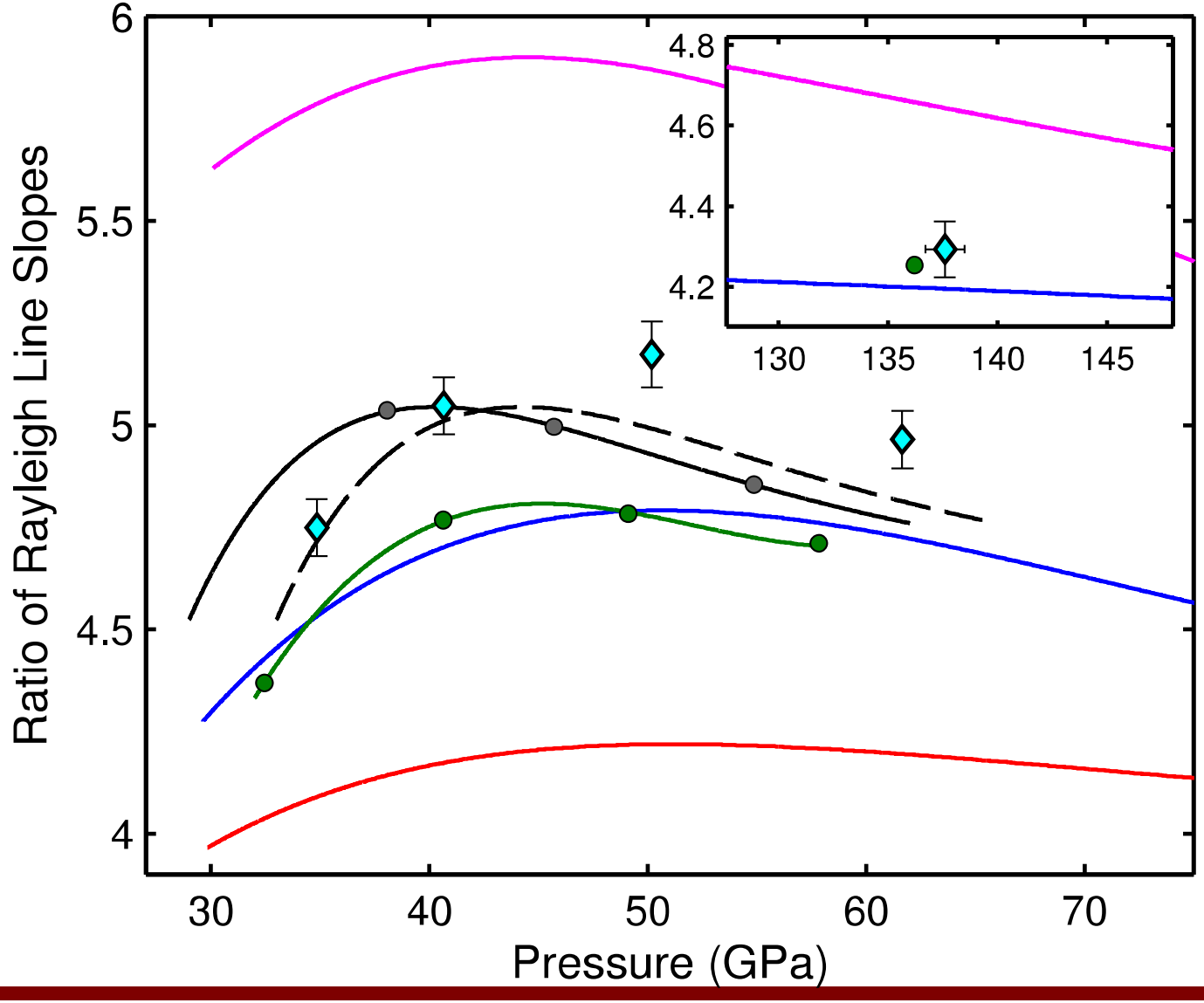
Recent results show significant improvement in precision with respect to previous data



Conclusions from Principal Hugoniot experiments are corroborated by reshock measurements



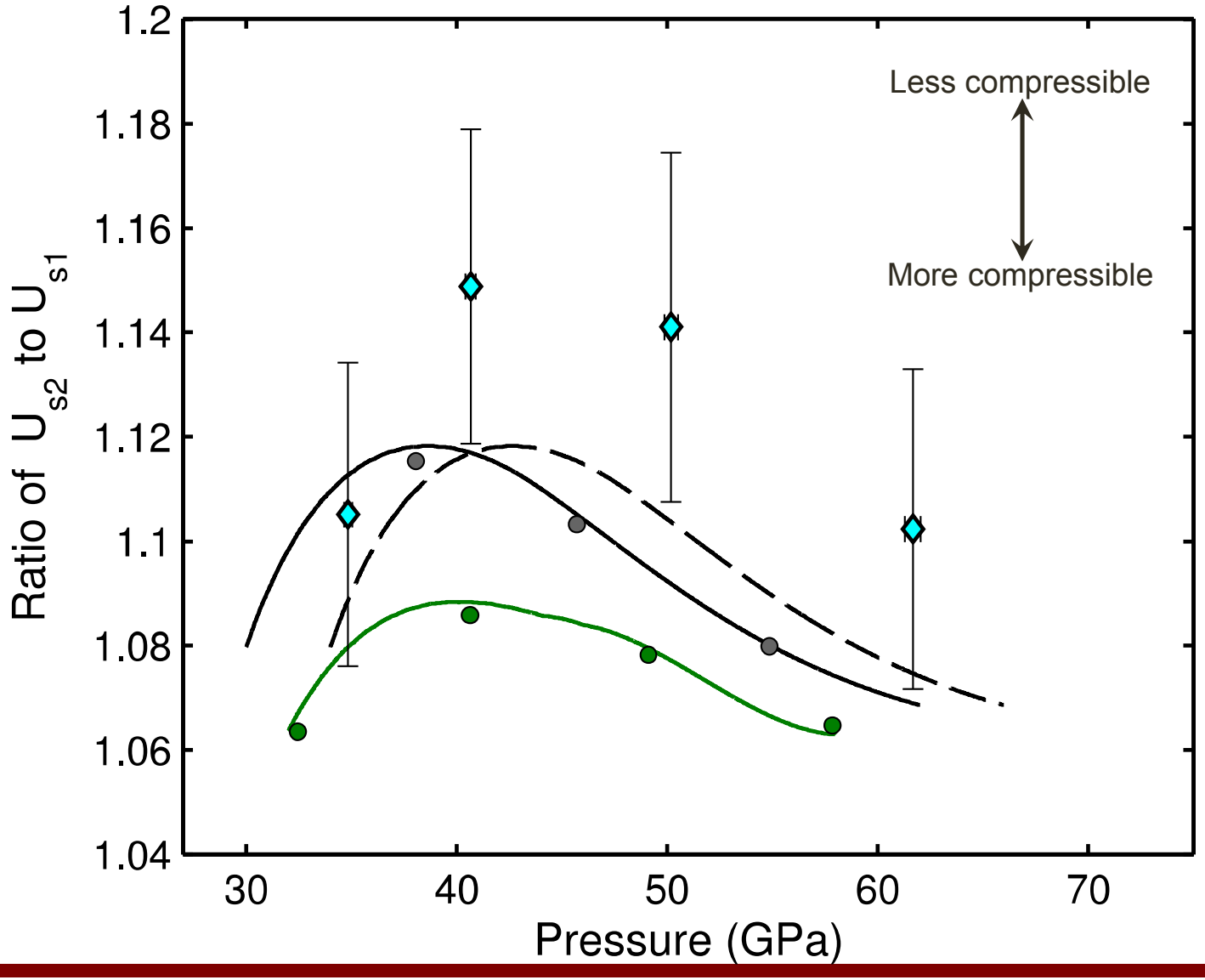
Conclusions from Principal Hugoniot experiments are corroborated by reshock measurements



Sesame72
Kerley03
Lenosky
PBE
PBE + 4 GPa
vdW-DF1
PBE
vdW-DF1
Z Quartz

$$\frac{R_2}{R_1} = \frac{\rho_1 U_{s_2}^D}{\rho_0 U_{s_1}^D}$$

Experimental reshock less compressible than DFT and is better described by PBE than DF1



Overall trend in the DFT results is consistent with experimental observations

Conclusions

- Shock-ramp technique enabled experimental access to the liquid-liquid, insulator-metal transition (LL-IMT)
- Experiments show clear evidence of metallization of deuterium
- Relative insensitivity to *T* at low temperature suggests this is a ρ-driven transition in the low temperature regime
  - ρ at the transition is inferred to be ~2-2.1 g/cc in deuterium
- Experiments at higher *T* in good agreement with previous work of Weir *et al.*
- High precision Hugoniot experiments enable evaluation of various quantum simulation methods
  - Experimental results do not agree with any one xc-functional
  - Perhaps best described by PBE with the understanding that the IMT occurs at ~3-4 GPa higher pressure than predicted by PBE

Acknowledgements

Experiment Design/Analysis

Marcus Knudson

Ray Lemke

Kyle Cochrane

Devon Dalton

Dustin Romero

Diagnostics

Charlie Meyer

Jeff Gluth

Devon Dalton

Anthony Romero

Dave Bliss

Alan Carlson

QMD Calculations

Mike Desjarlais

Andreas Becker

Winfried Lorenzen

Ronald Redmer

Planetary Modeling

Nadine Nettelmann

Andreas Becker

Ronald Redmer

Pulse Shaping

Ray Lemke

Jean-Paul Davis

Mark Savage

Ken Struve

Keith LeChien

Brian Stoltzfus

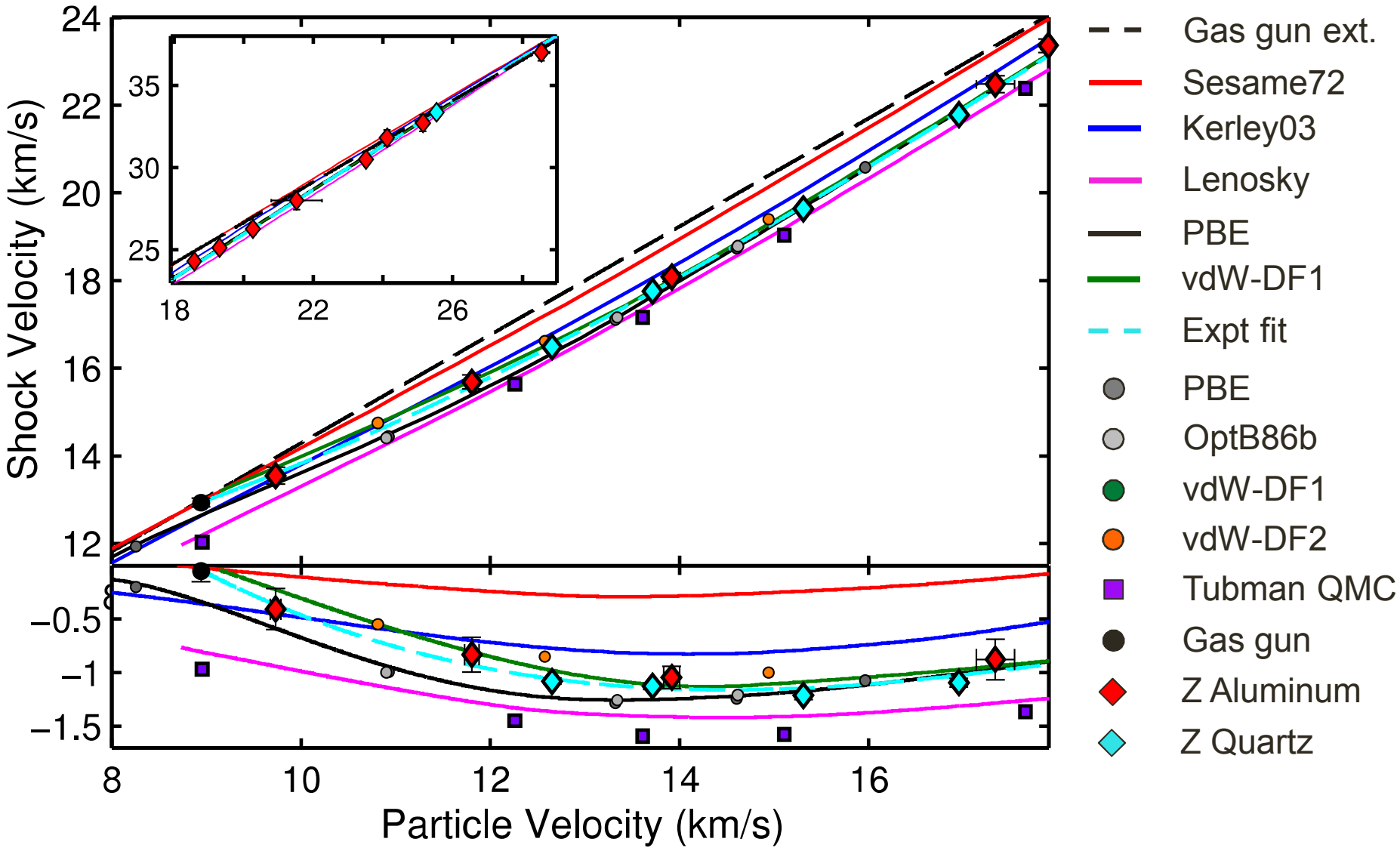
Dave Hinshelwood

Entire Z crew

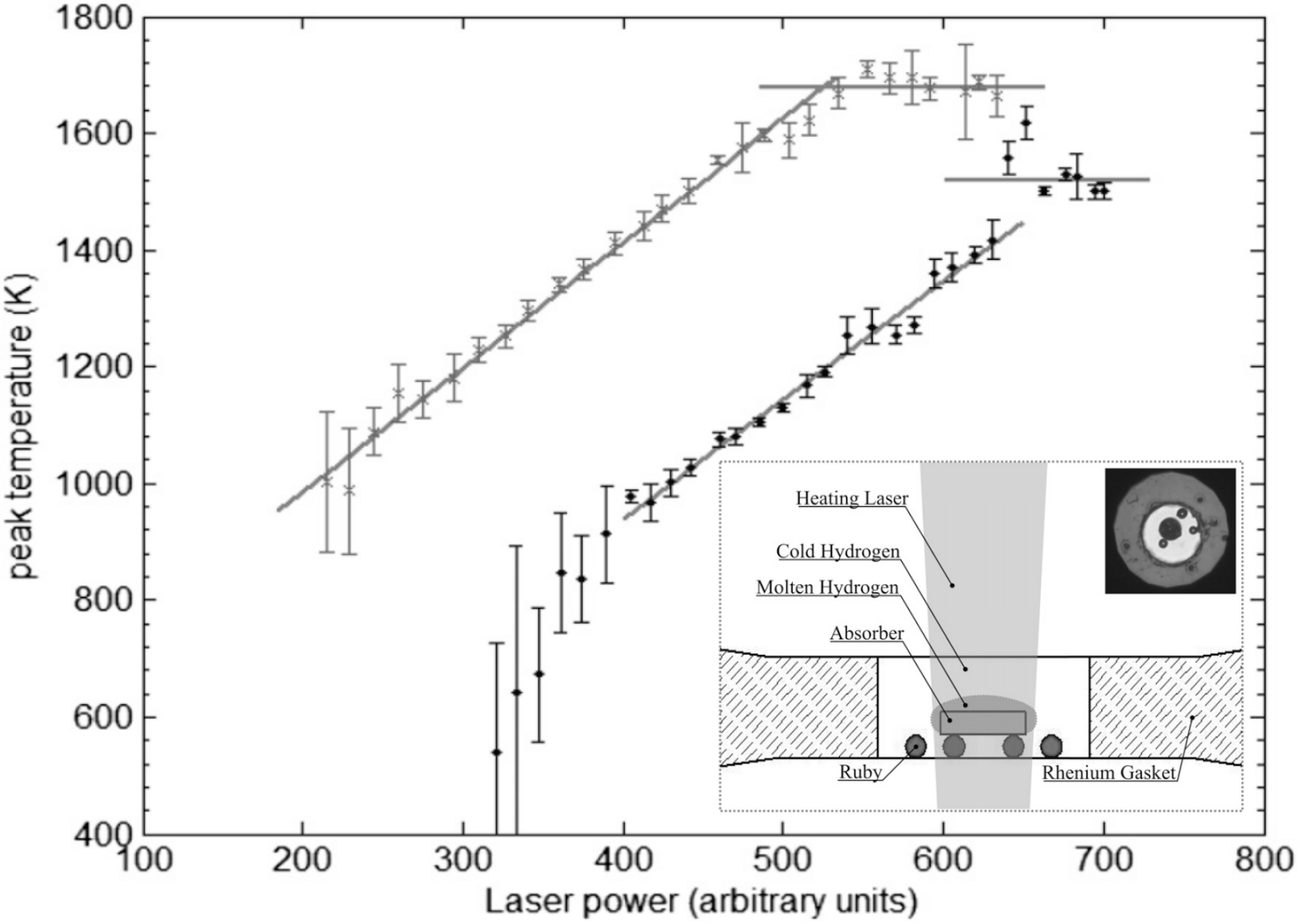
University of Rostock

Back-Ups

Recent results show significant improvement in precision with respect to previous data

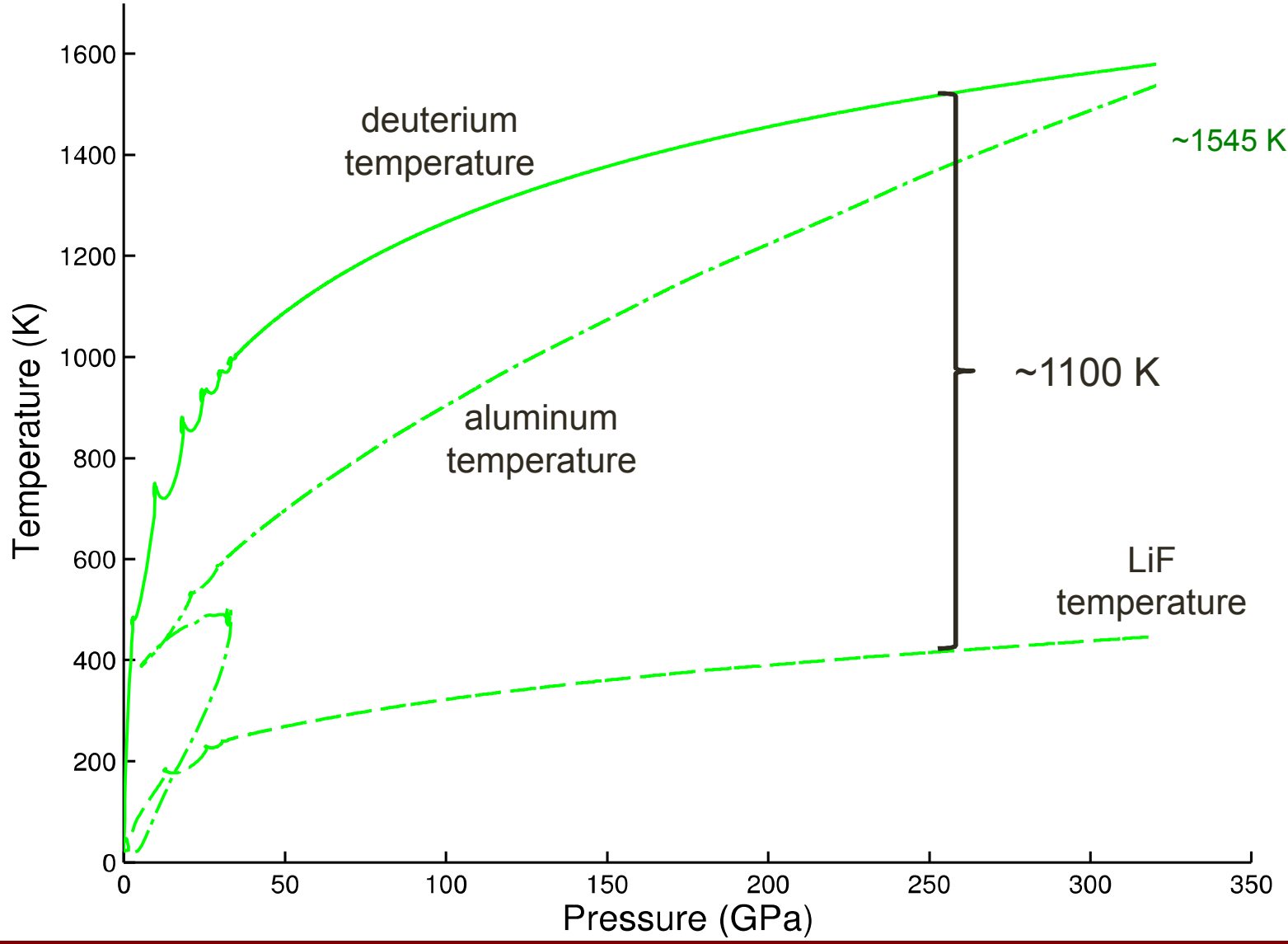


Dzyabura experiment

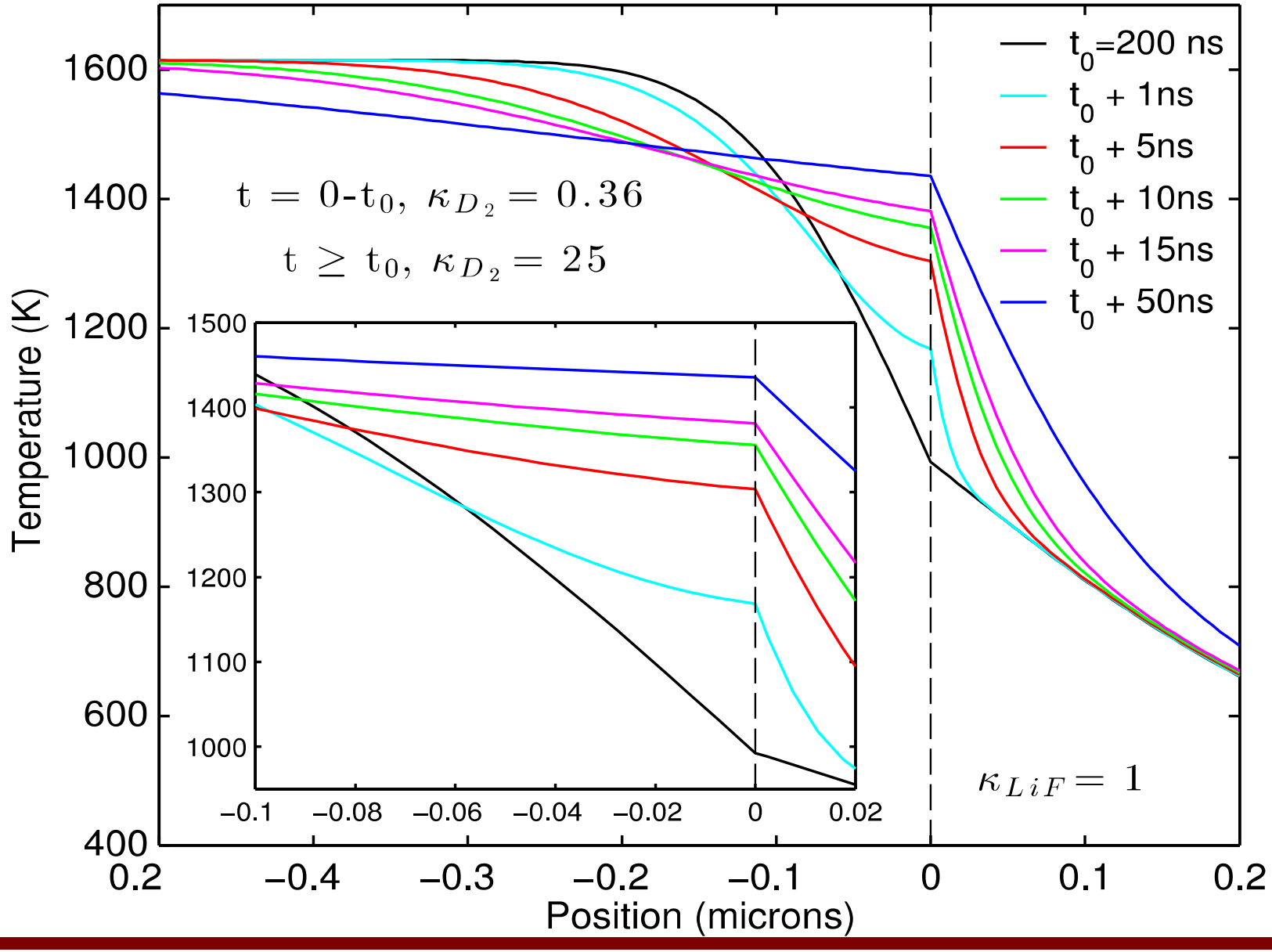


V. Dzyabura, et al. Proc. Natl. Acad. Sci. U.S.A. 110, 8040 (2013)

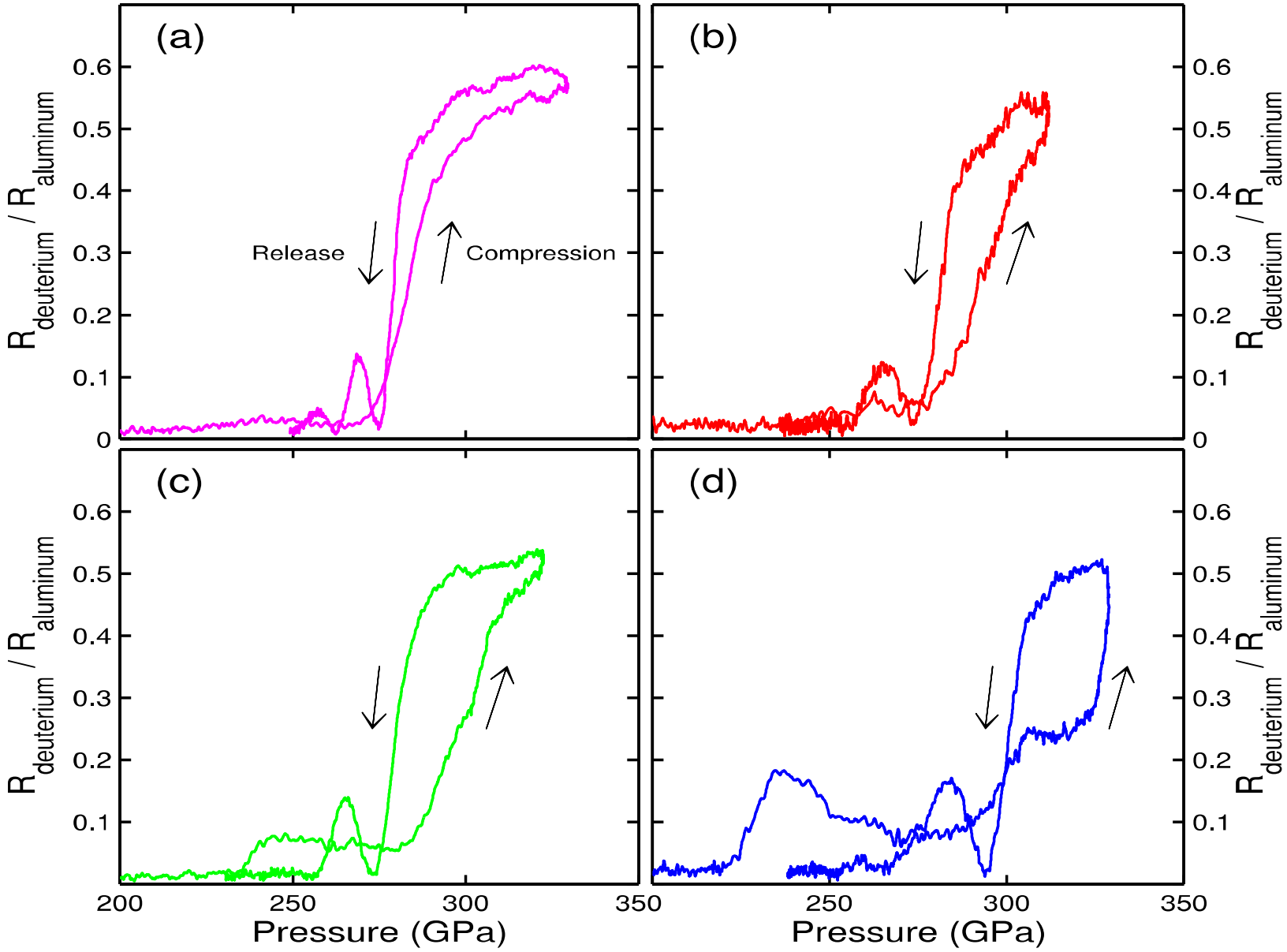
There is a significant temperature difference at the deuterium/LiF interface



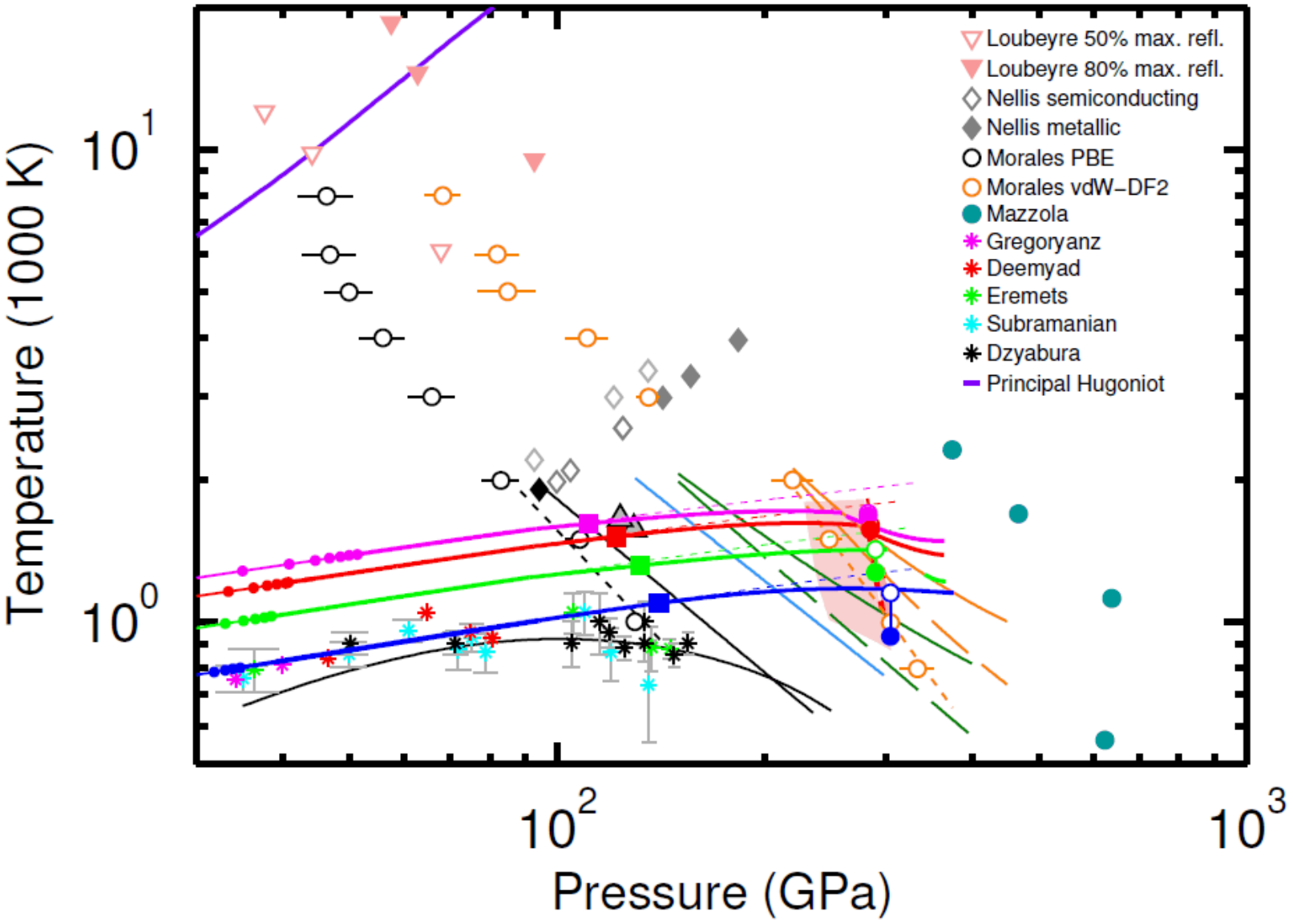
Thermal conduction simulations



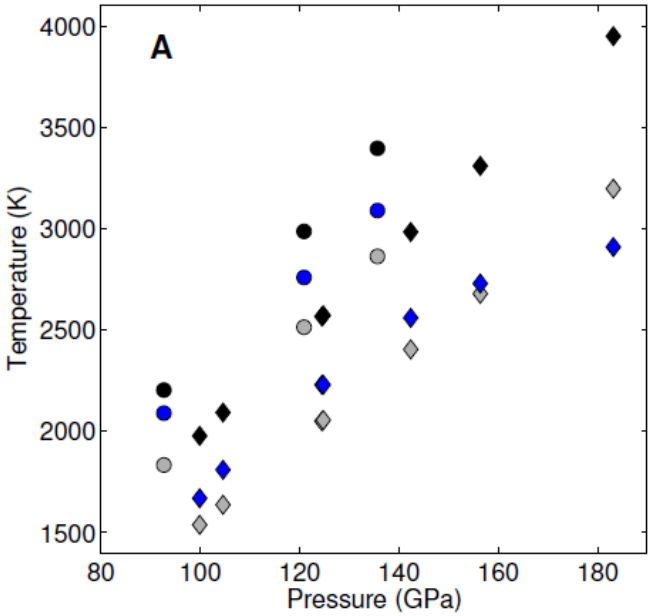
Reflectivity signals mapped to pressure

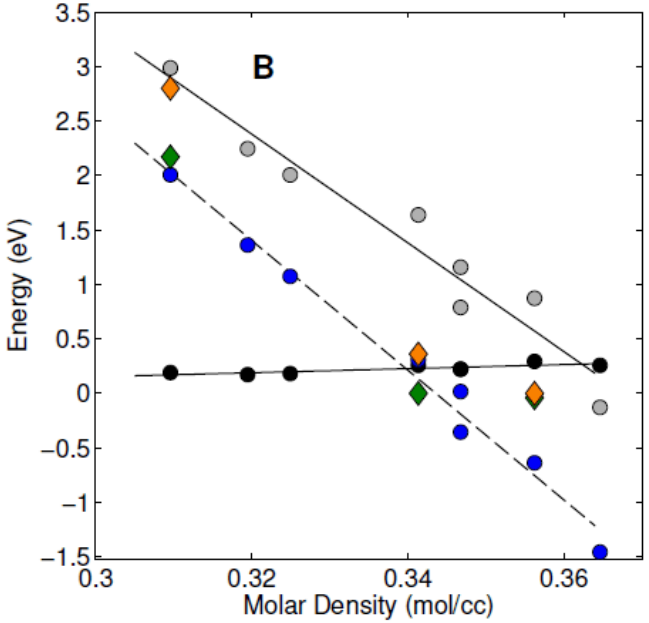


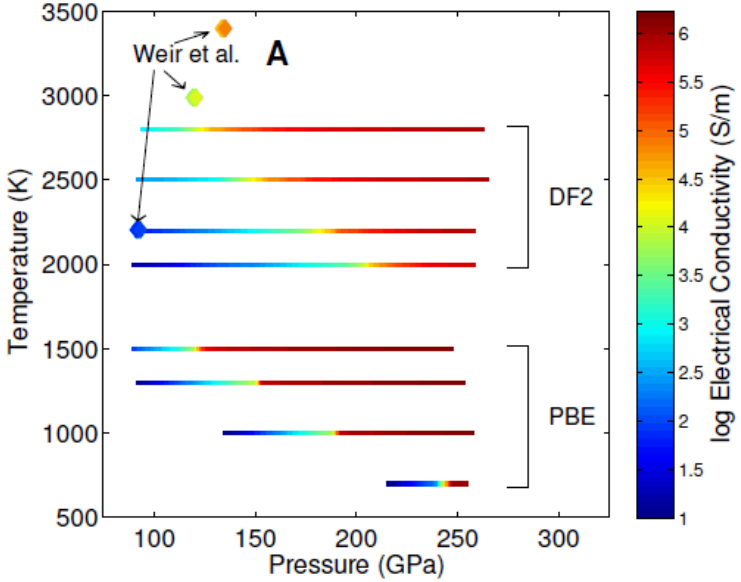
Extended P-T diagram for hydrogen

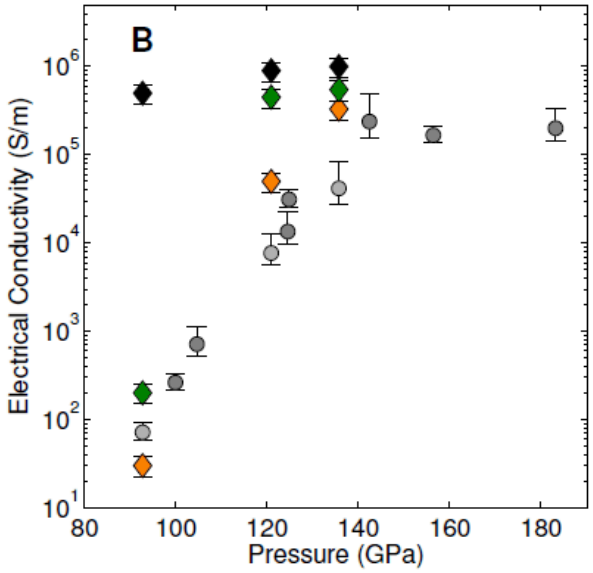


Reanalysis of Weir et al data

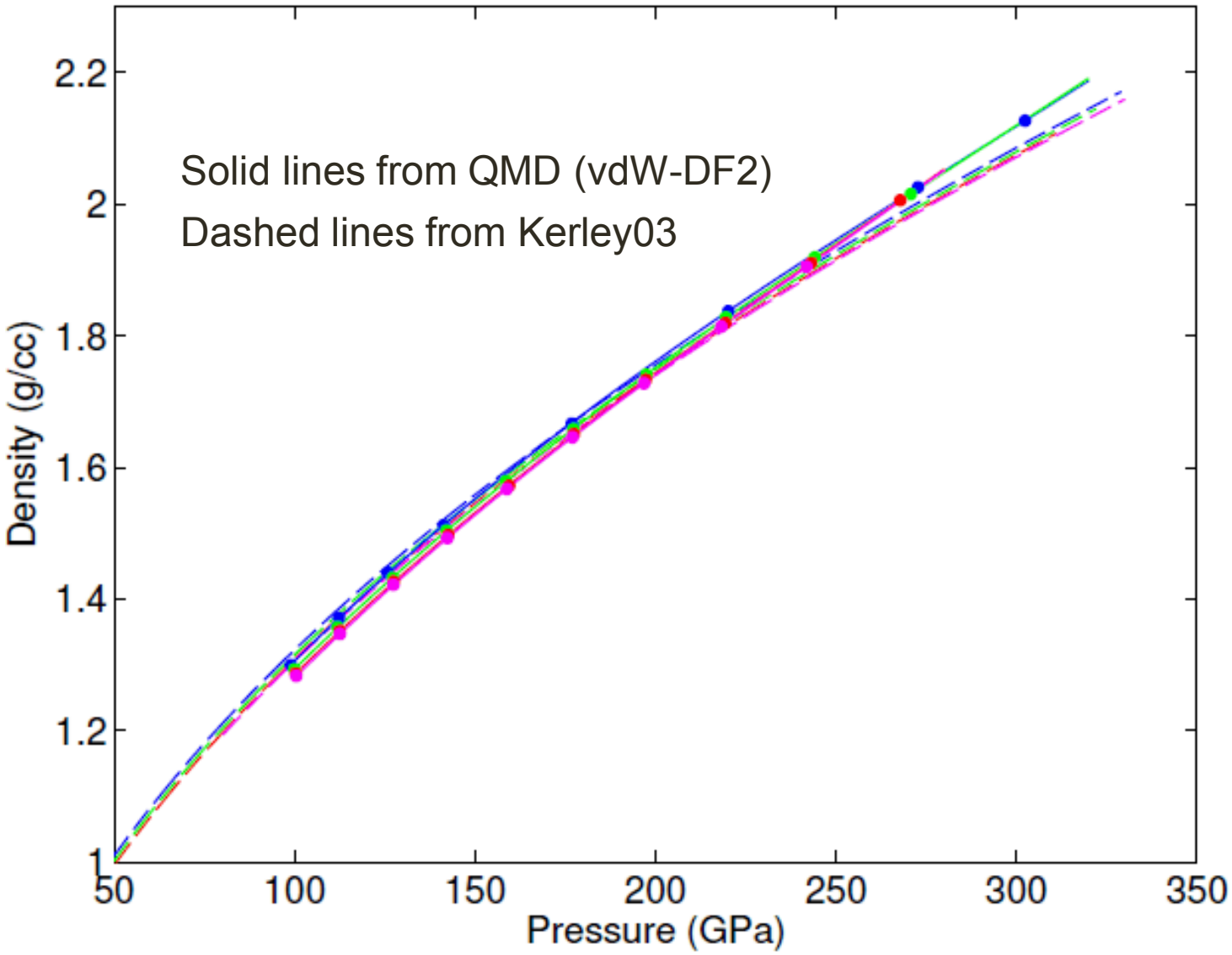






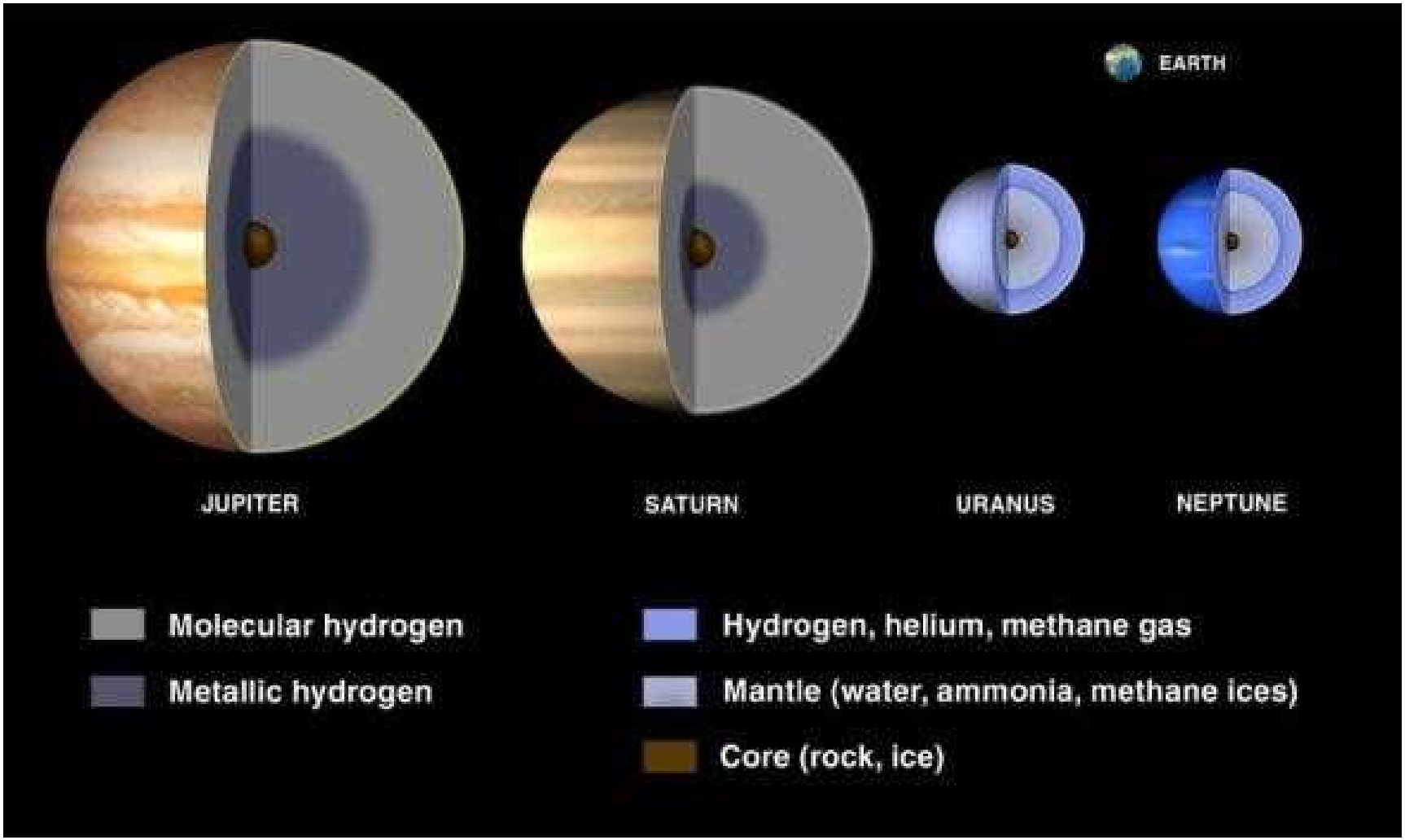


P(ρ) relatively insensitive to EOS model

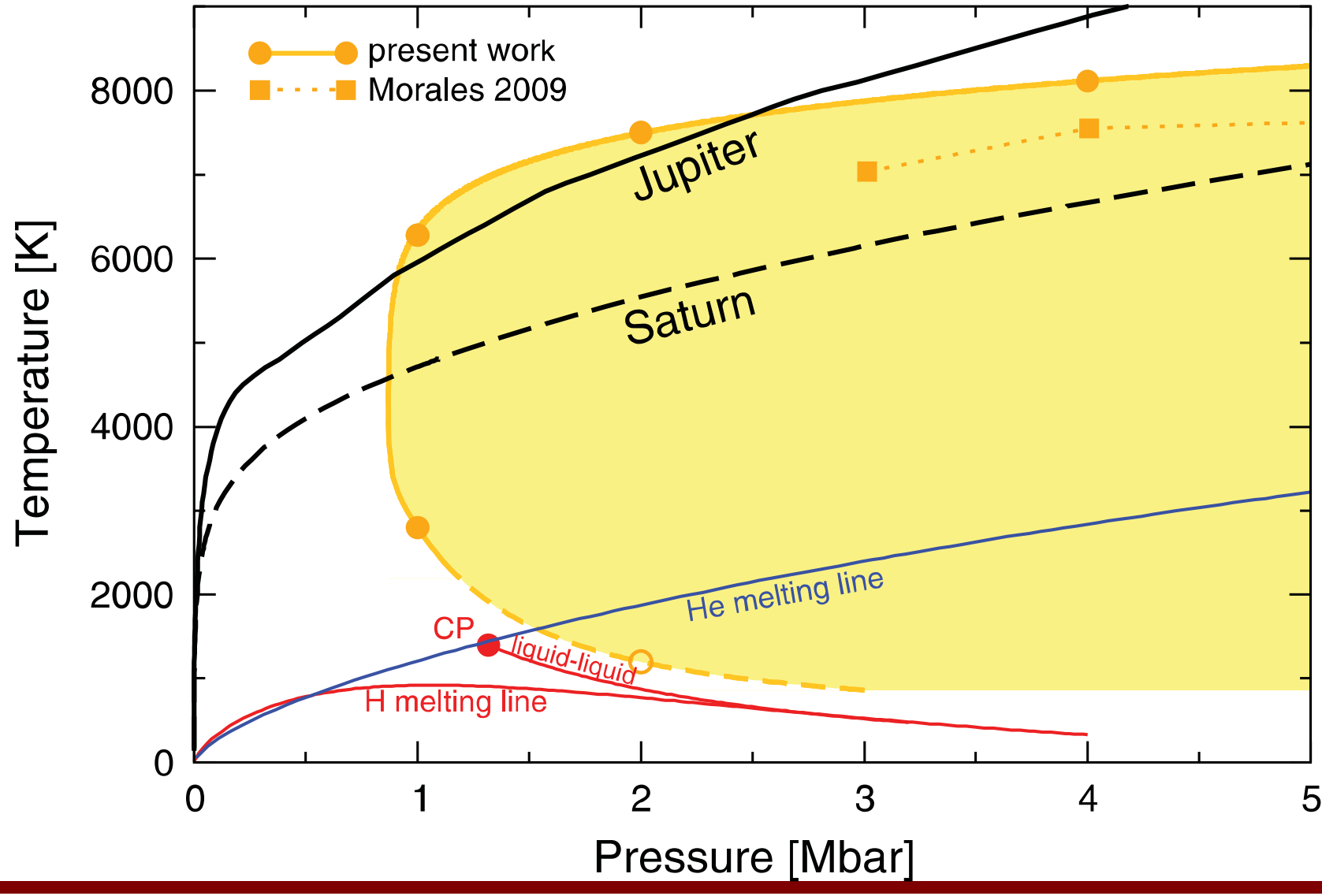


Giant planets in the Solar system

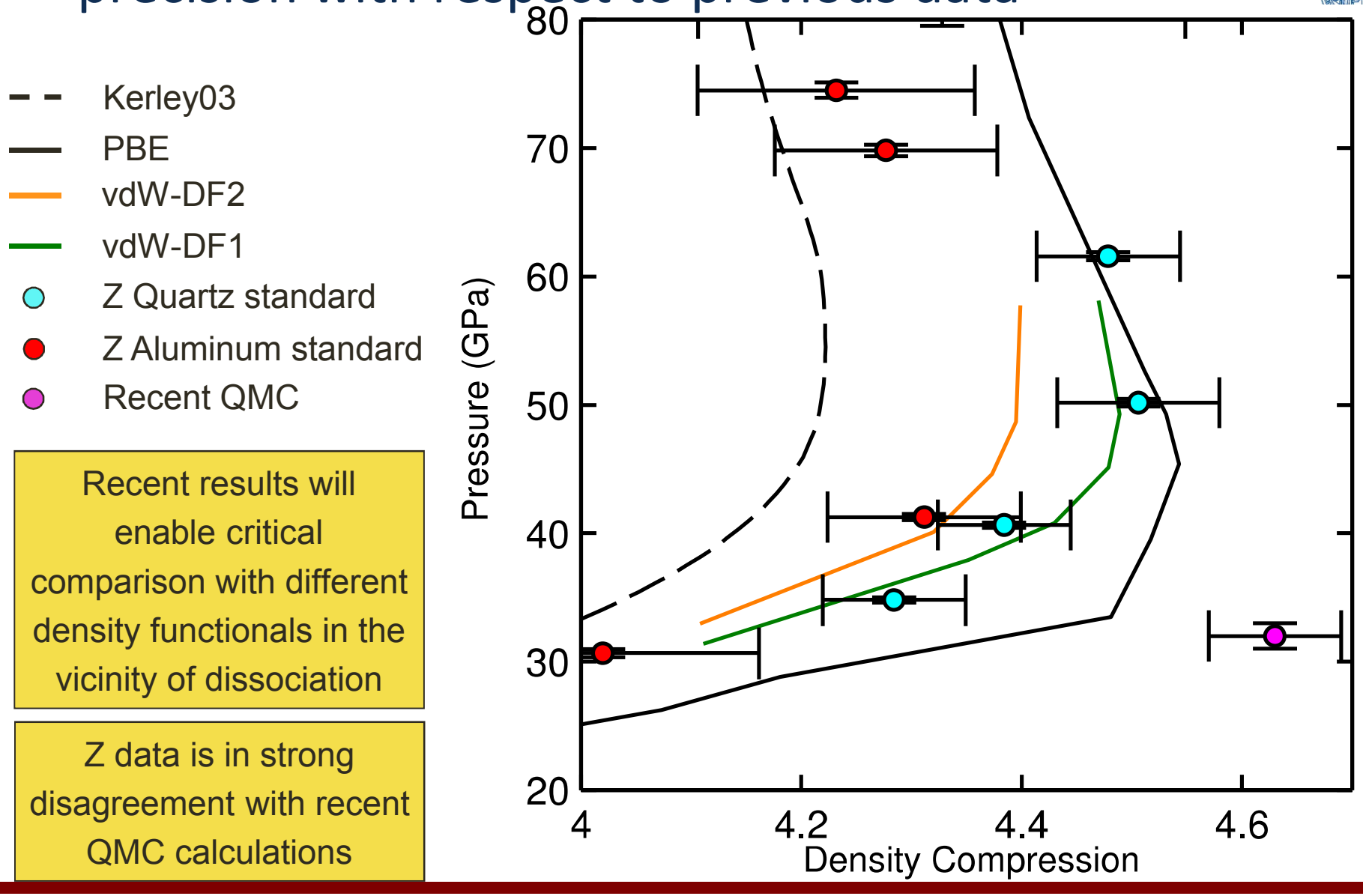
Interior composed of the lightest elements H & He, hydrides NH_3, OH_2, CH_4 (ices) and small amounts of heavier elements (cores)



H-He de-mixing appears to be precipitated at low T and P by metallization in hydrogen



Recent results show significant improvement in precision with respect to previous data

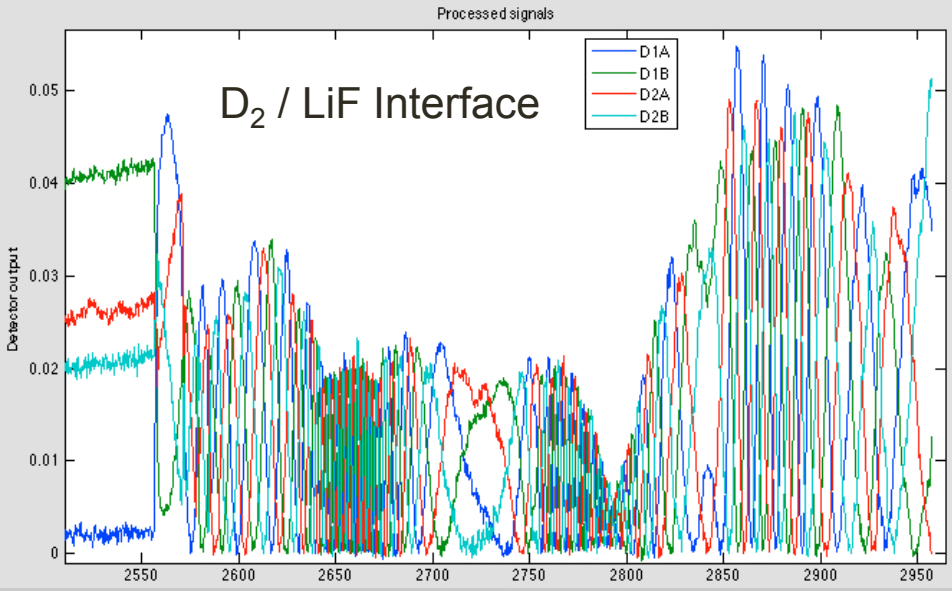


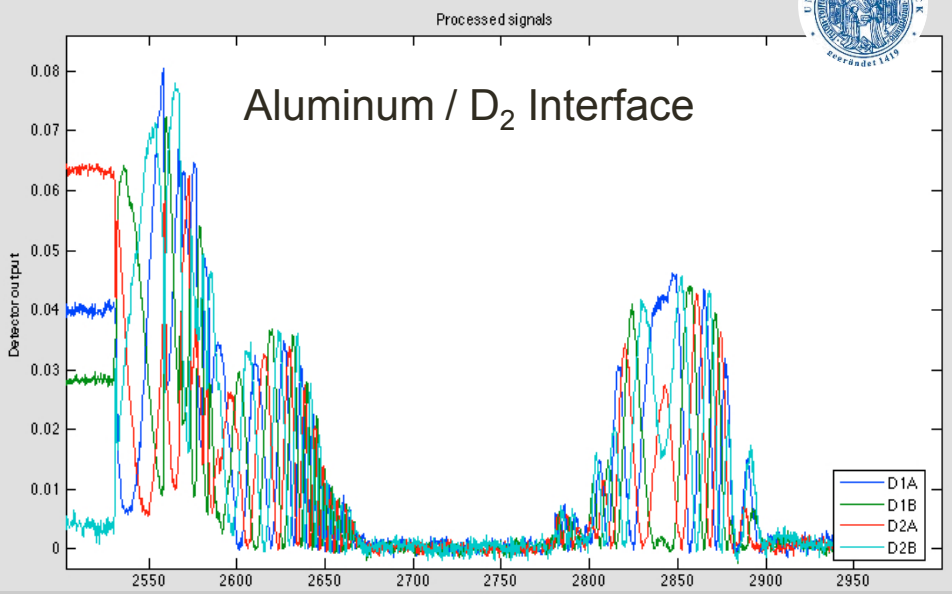
Recent results will enable critical comparison with different density functionals in the vicinity of dissociation

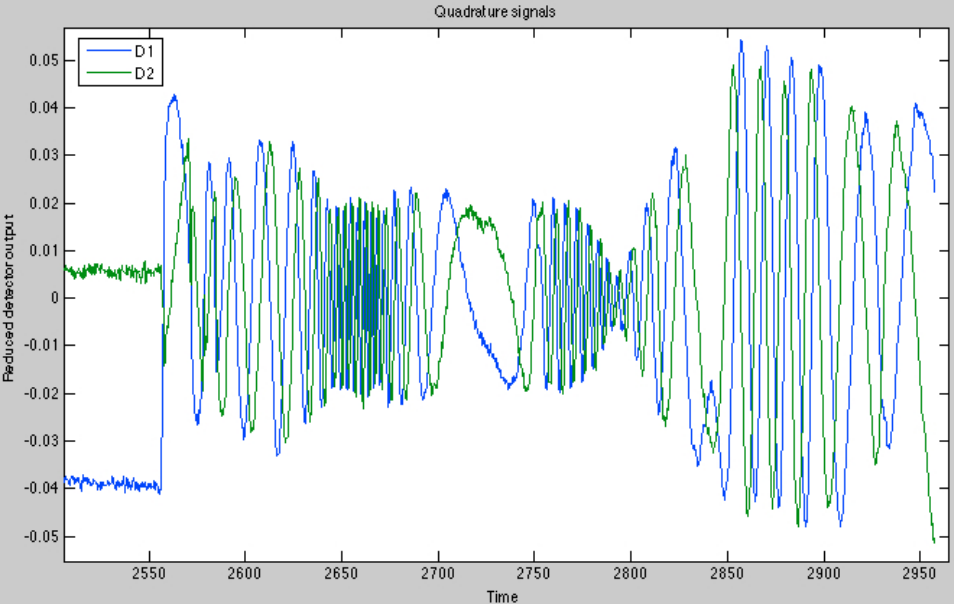
Z data is in strong disagreement with recent QMC calculations

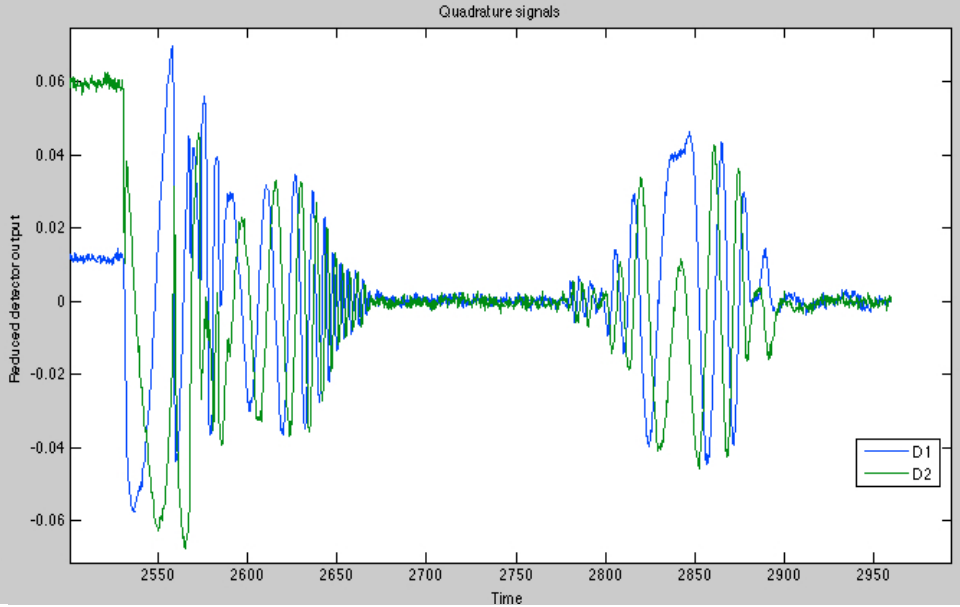
Tubman et al., PRL 115, 045301 (2015) Knudson et al., PRB 69, 144209 (2004) Desjarlais, PRB 68, 064204 (2003)

Processed VISAR signals









Stripline experimental profiles