SAND2016-4607C

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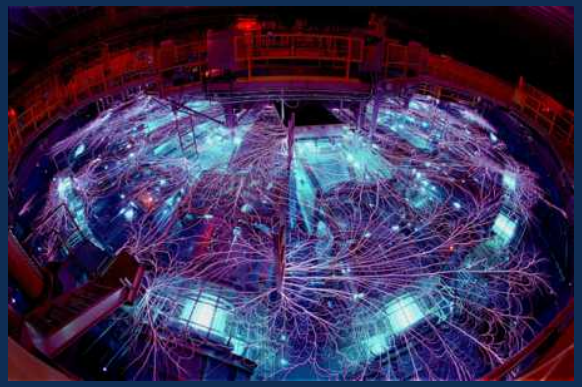
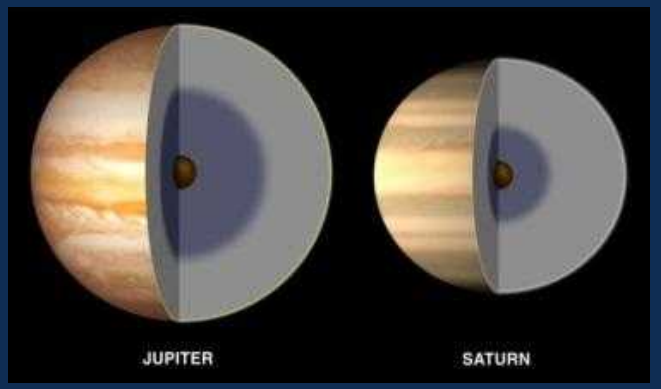




Dynamic compression experiments on deuterium and their implications for first-principles theory

Marcus D. Knudson

mdknuds@sandia.gov

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

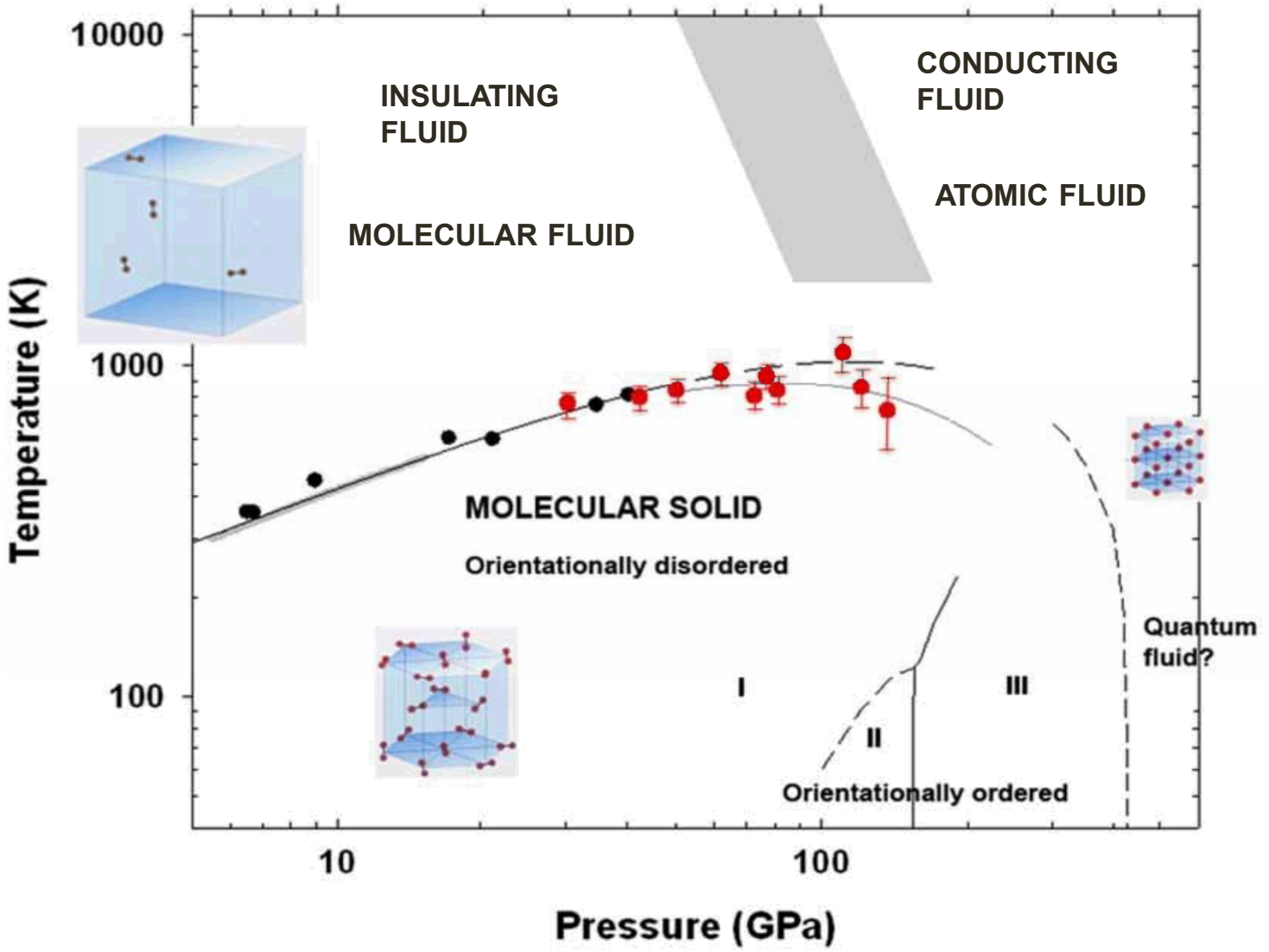
Brian Stoltzfus

Dave Hinshelwood

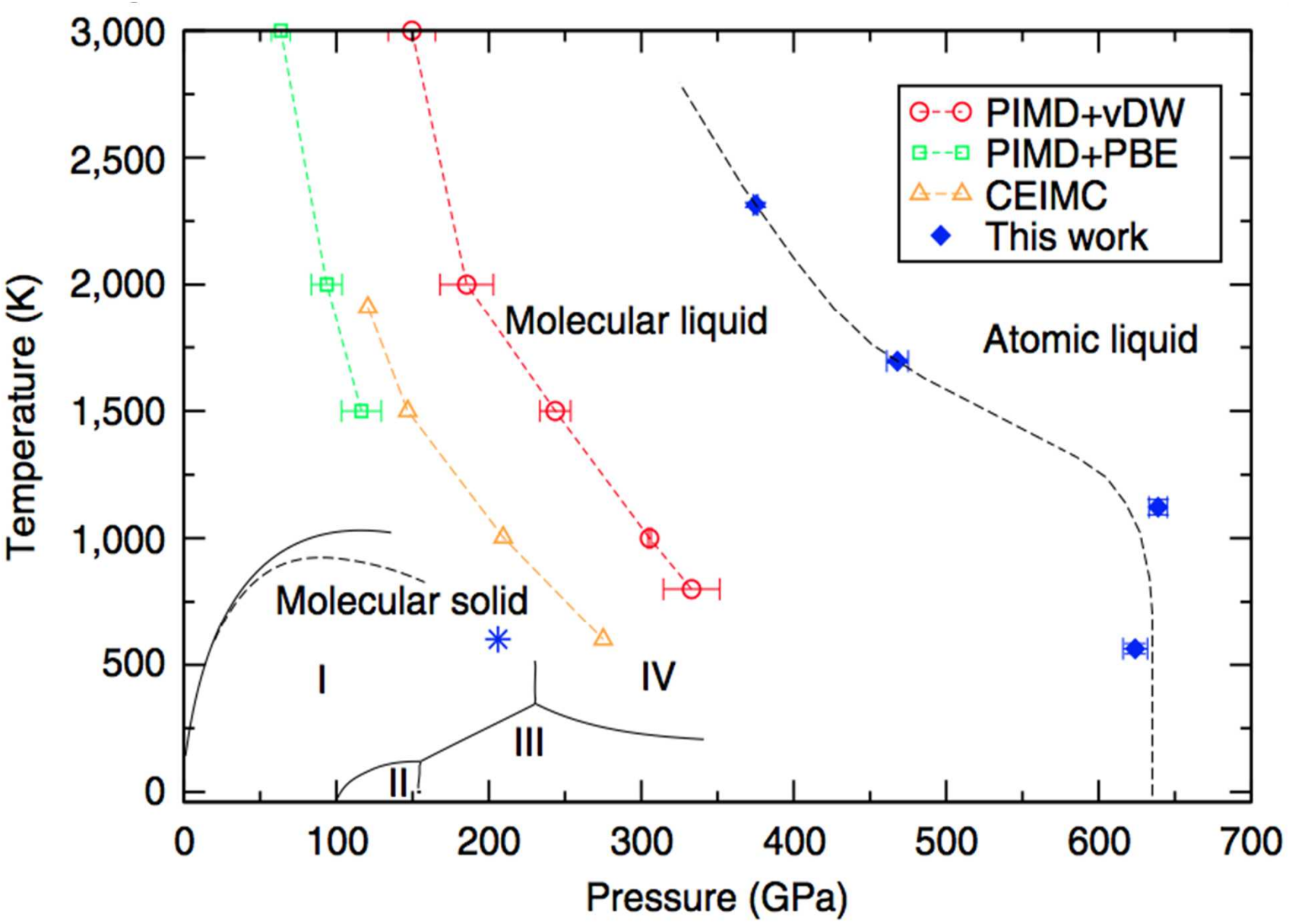
Entire Z crew

University of Rostock

Hydrogen at high pressures – the known phase diagram so far



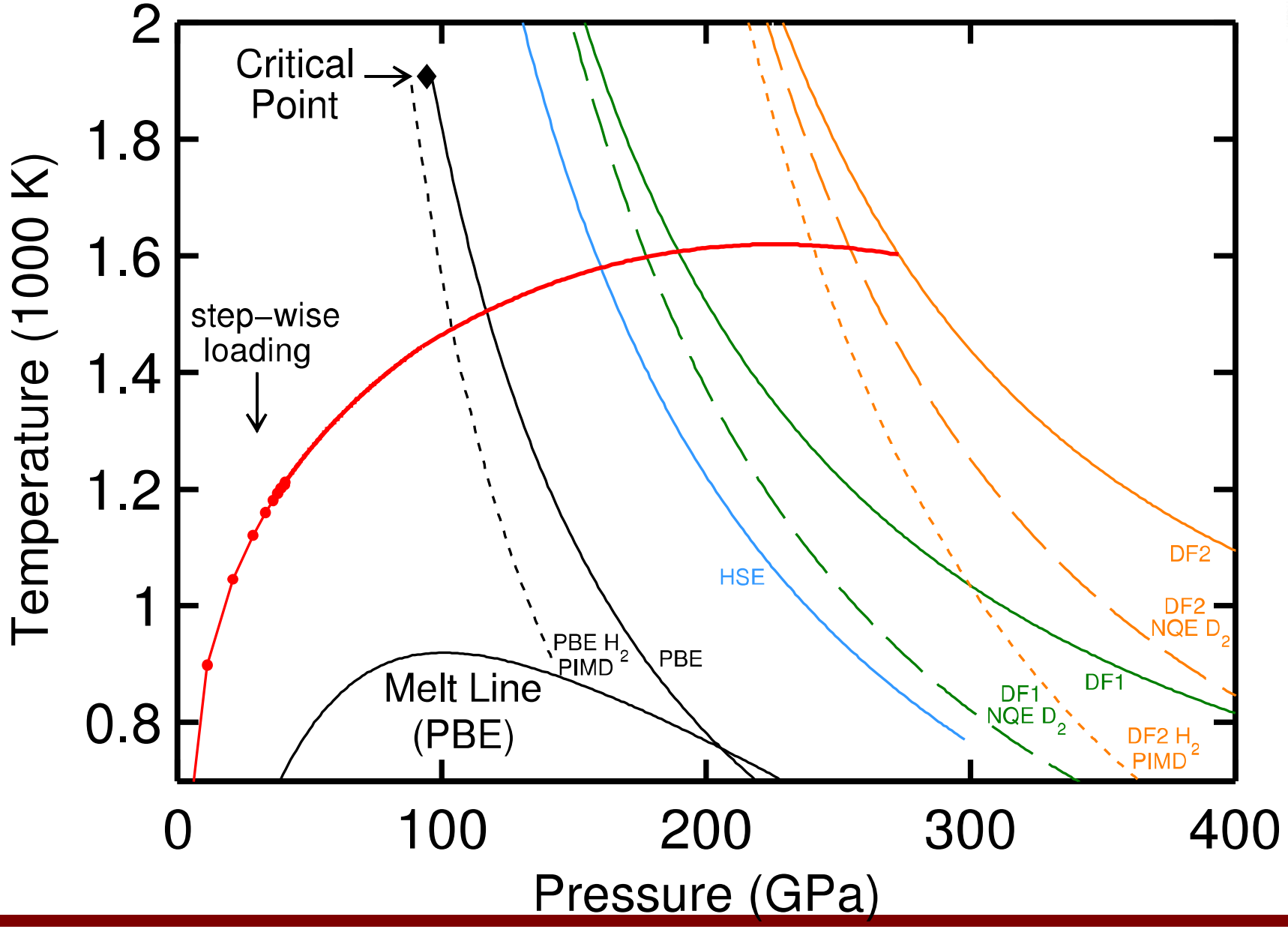
Recent predictions of the LL-IMT in hydrogen



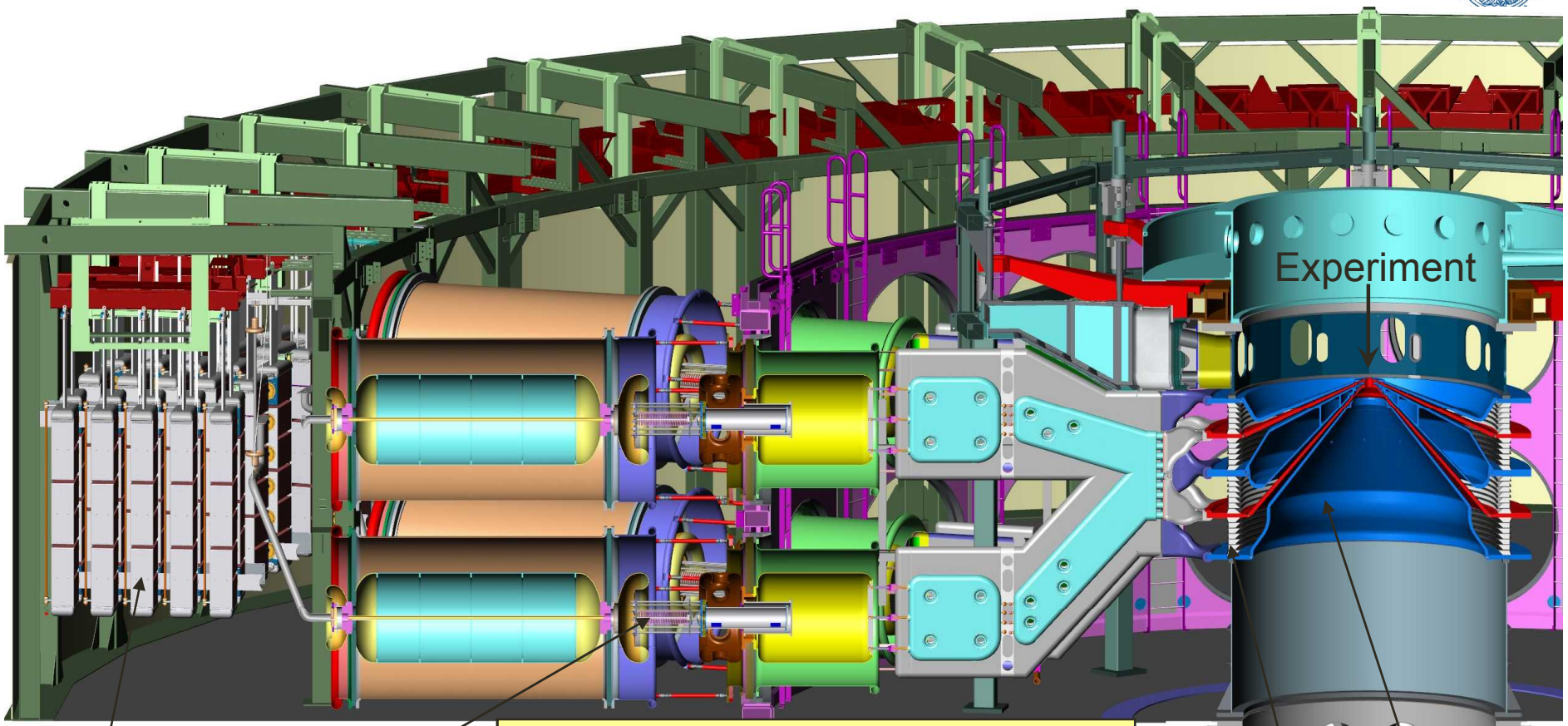
W. Lorenzen et al. Phys. Rev. B 82, 195107 (2010)
V. Morales et al. Proc. Natl. Acad. Sci. 107, 12799 (2010)
M. Morales et al. Phys. Rev. Lett. 110, 065702 (2013)

Dense Matter (2014)

Proposed Experiment: Shock - Ramp



Sandia Z Machine

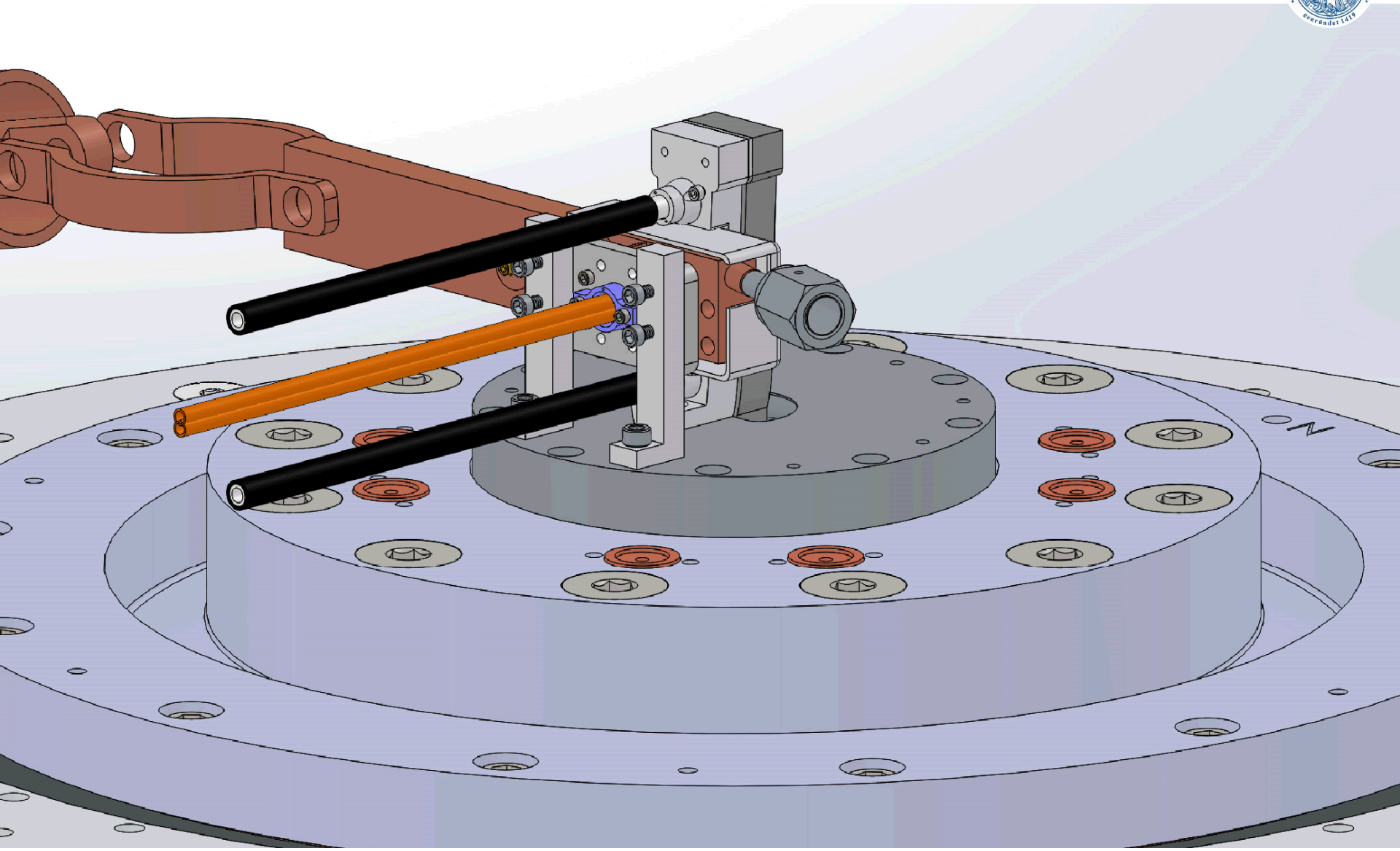


22 MJ stored energy

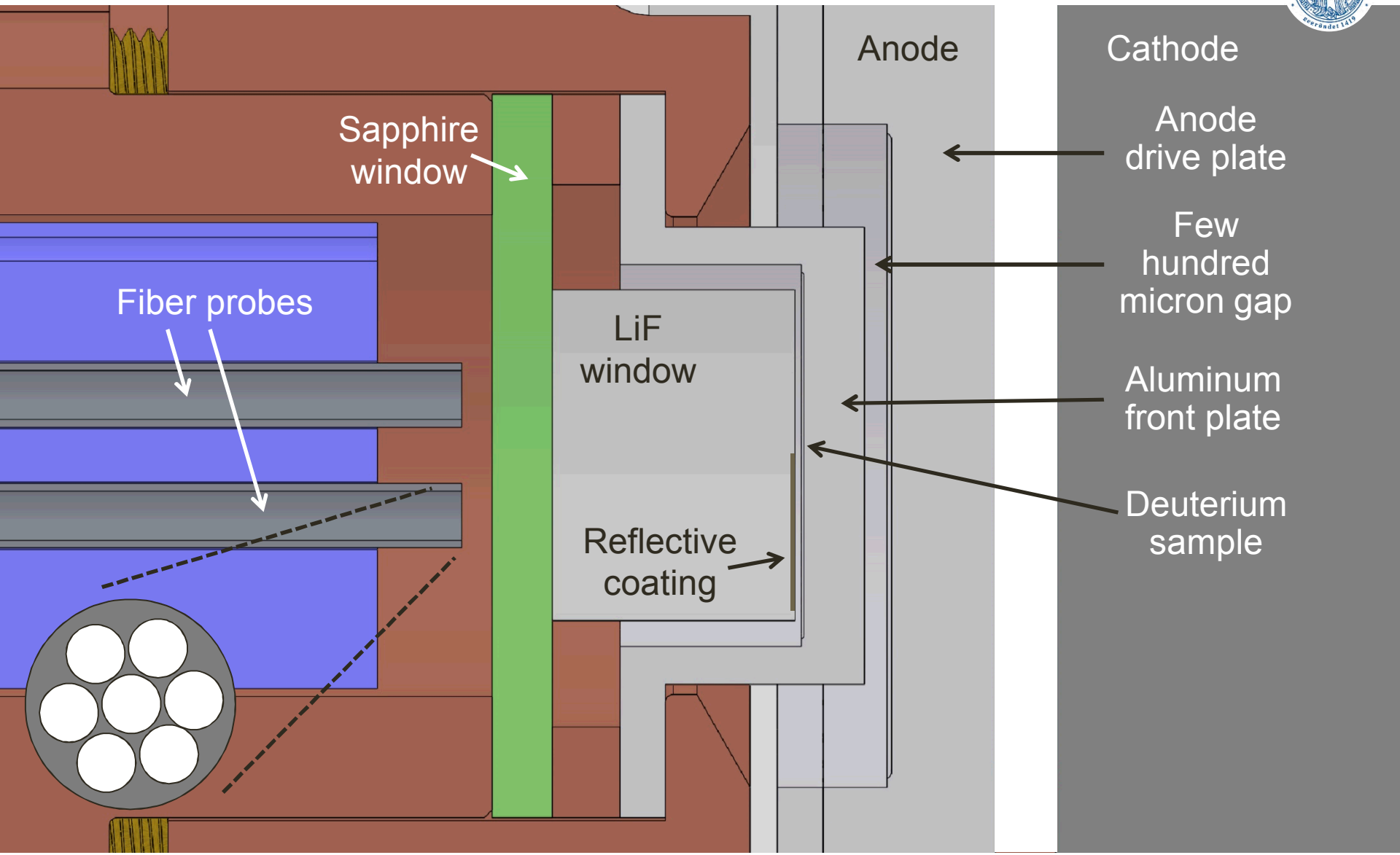
~25 MA peak current

~200-600 ns rise time

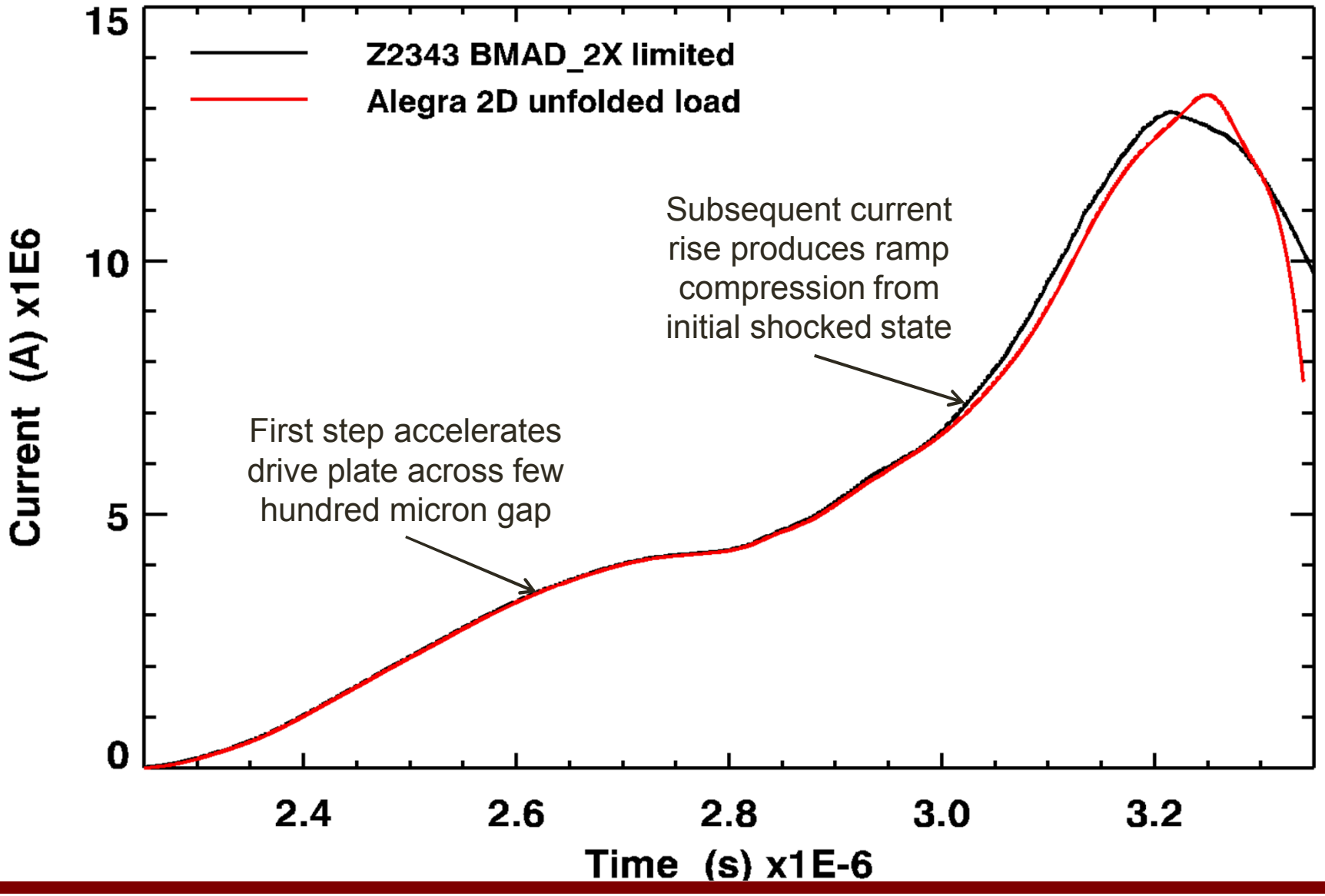
Stripline experimental configuration



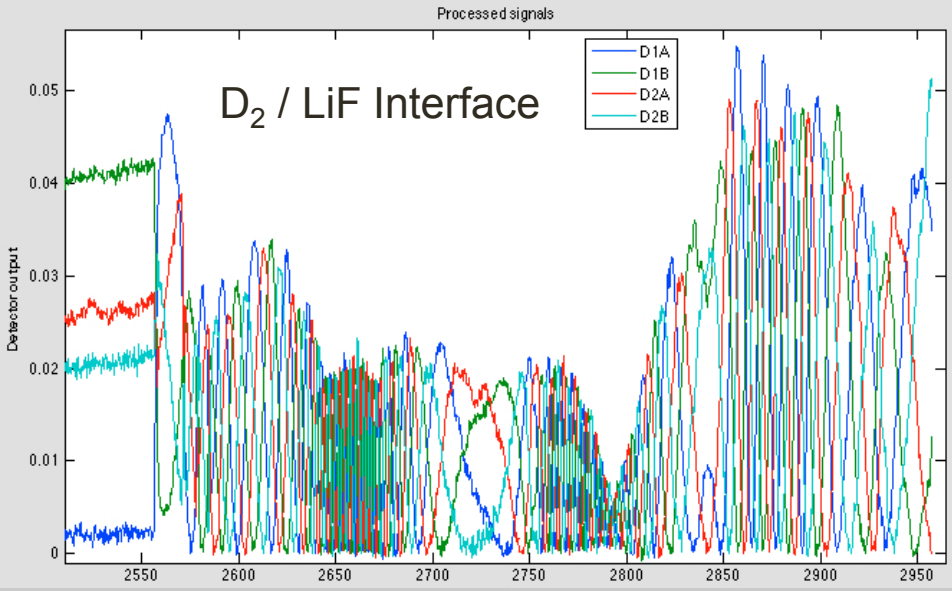
Experimental configuration

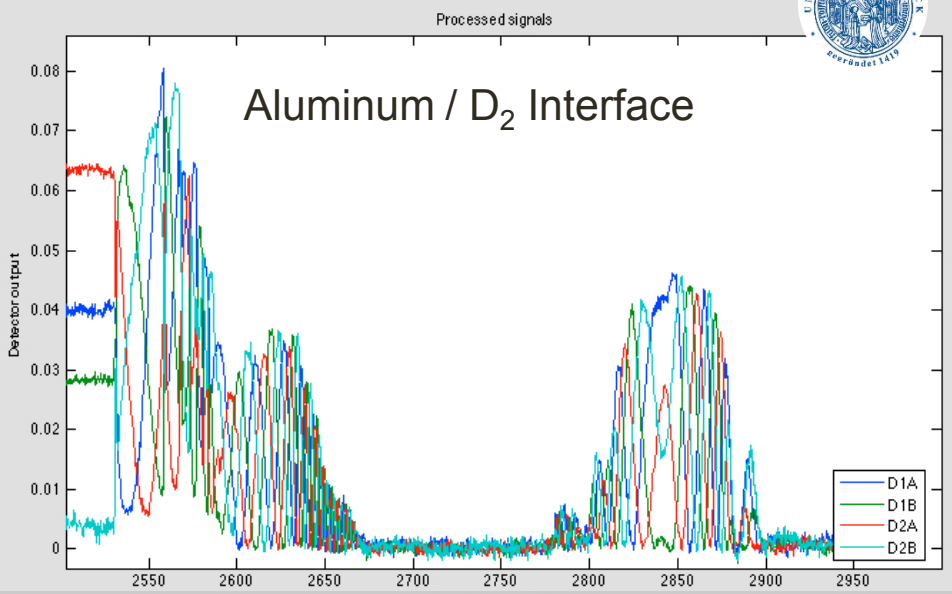


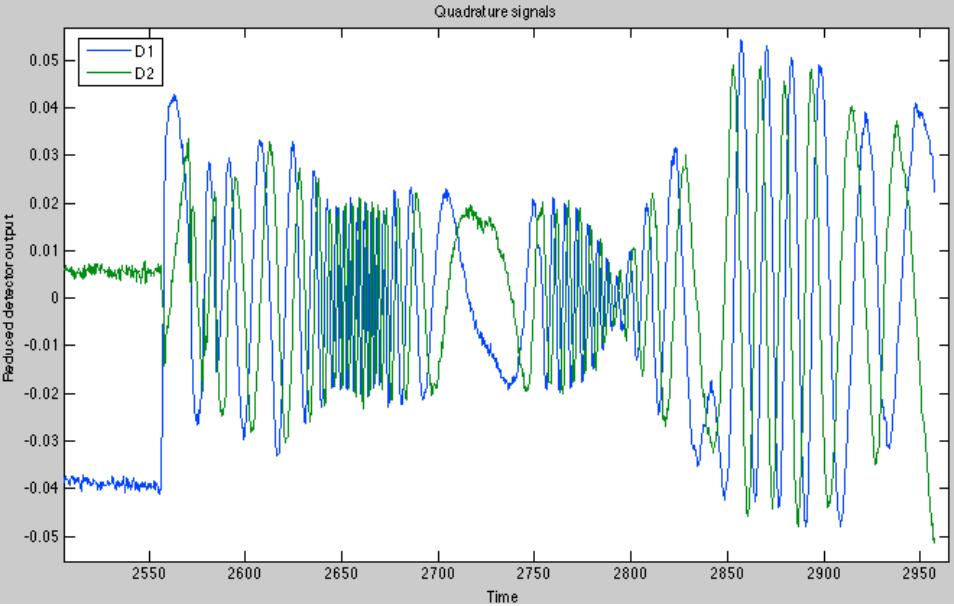
Two-step pulse shape provides shock-ramp profile

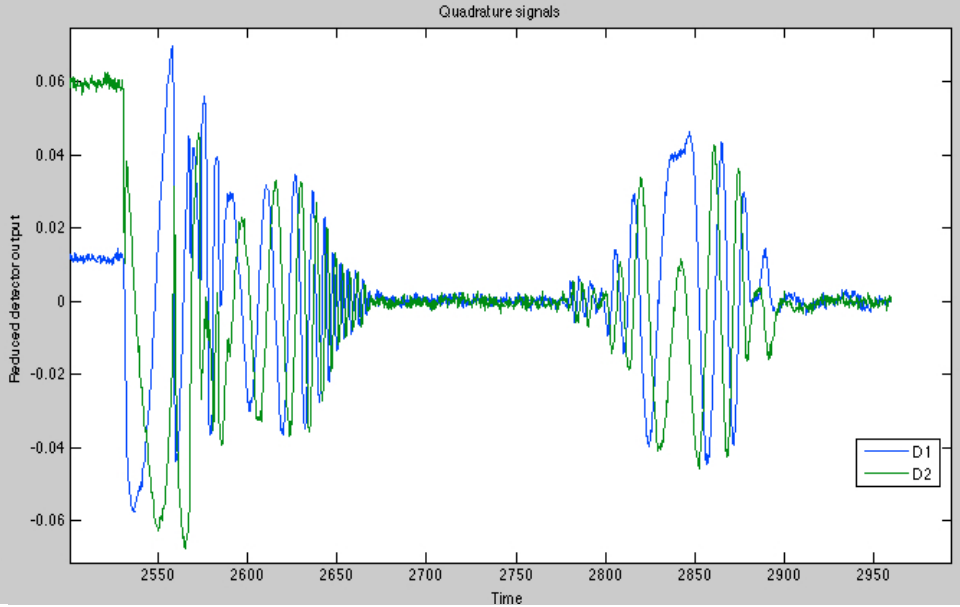


Processed VISAR signals

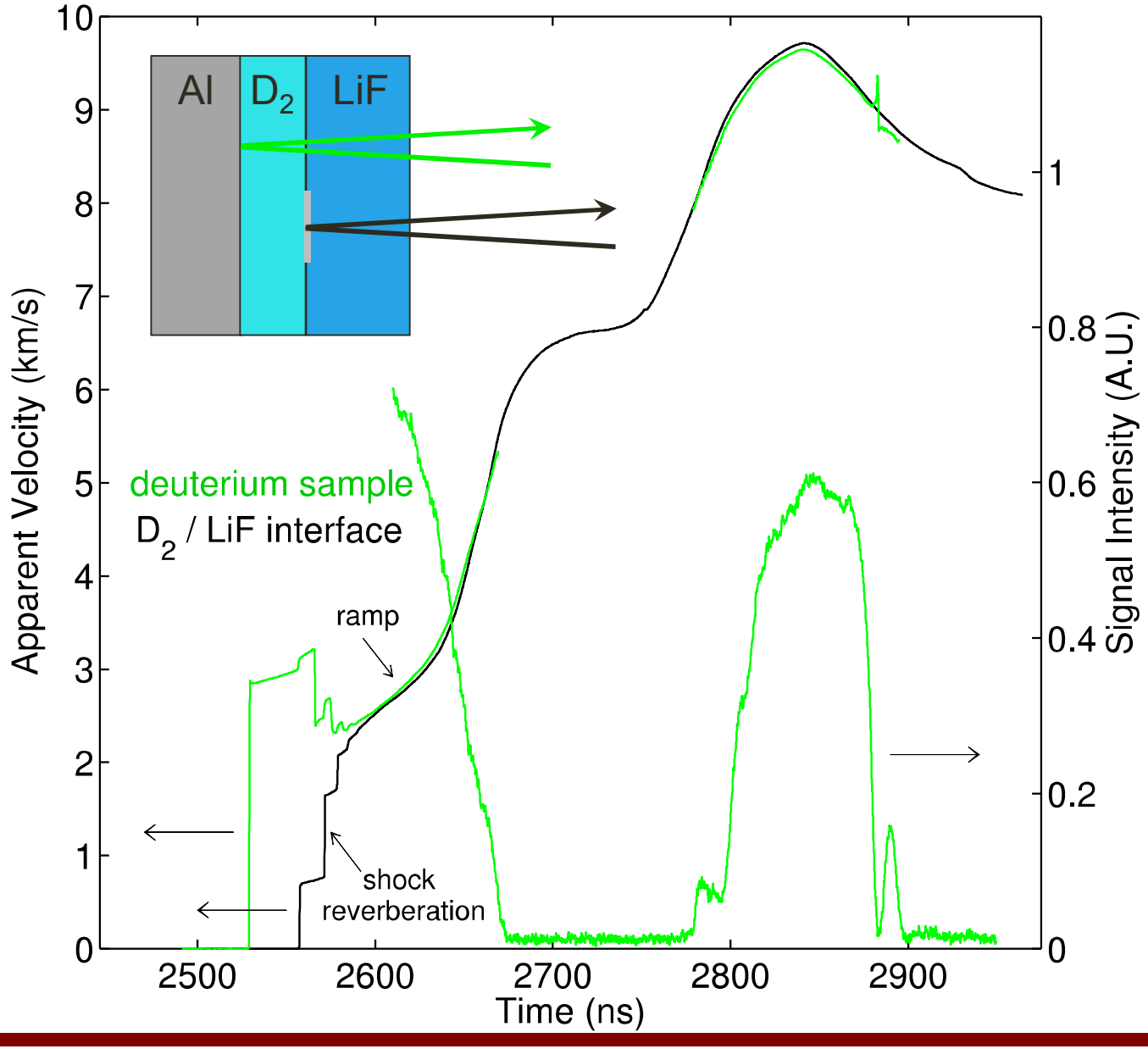




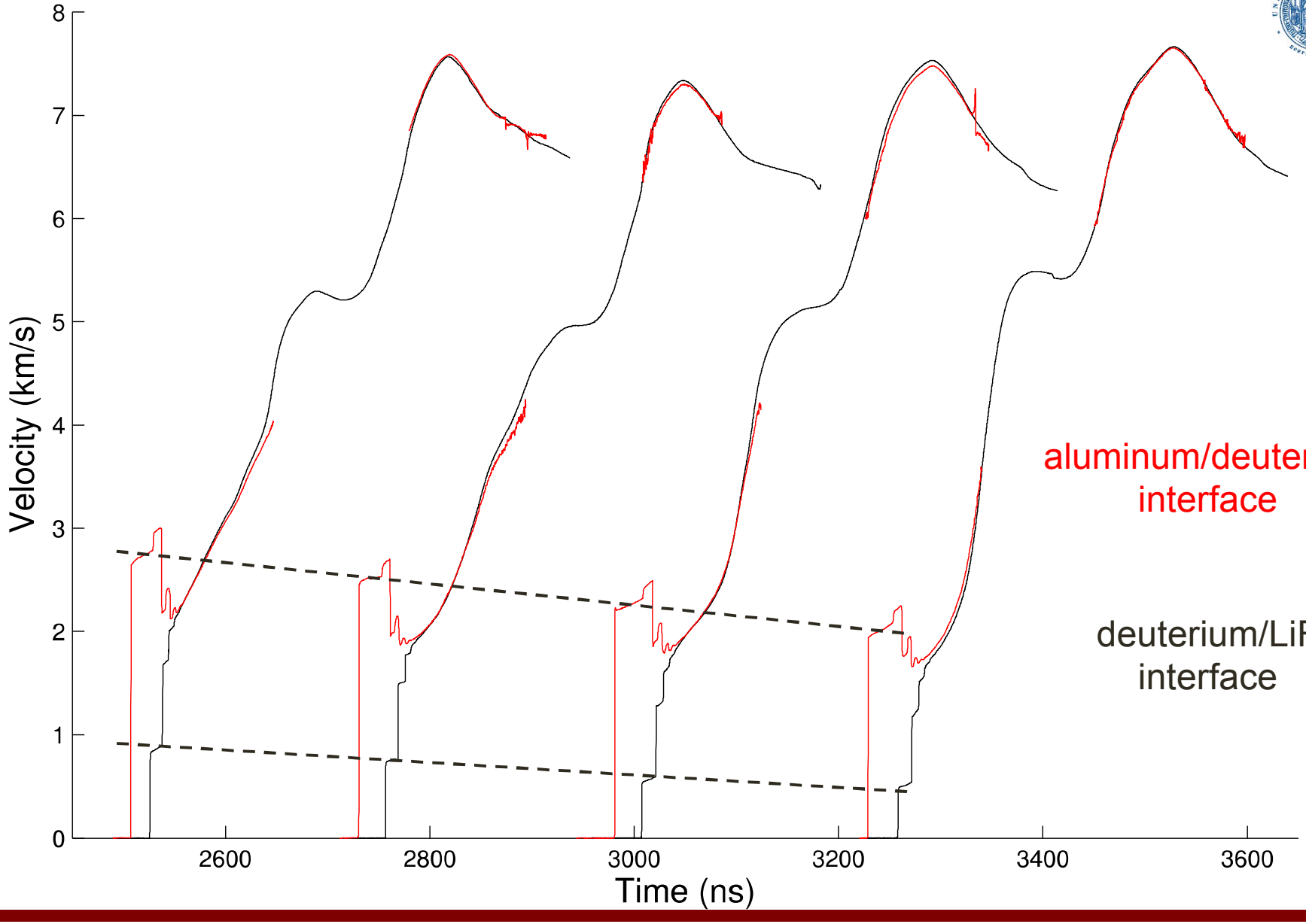




Measured observables in deuterium



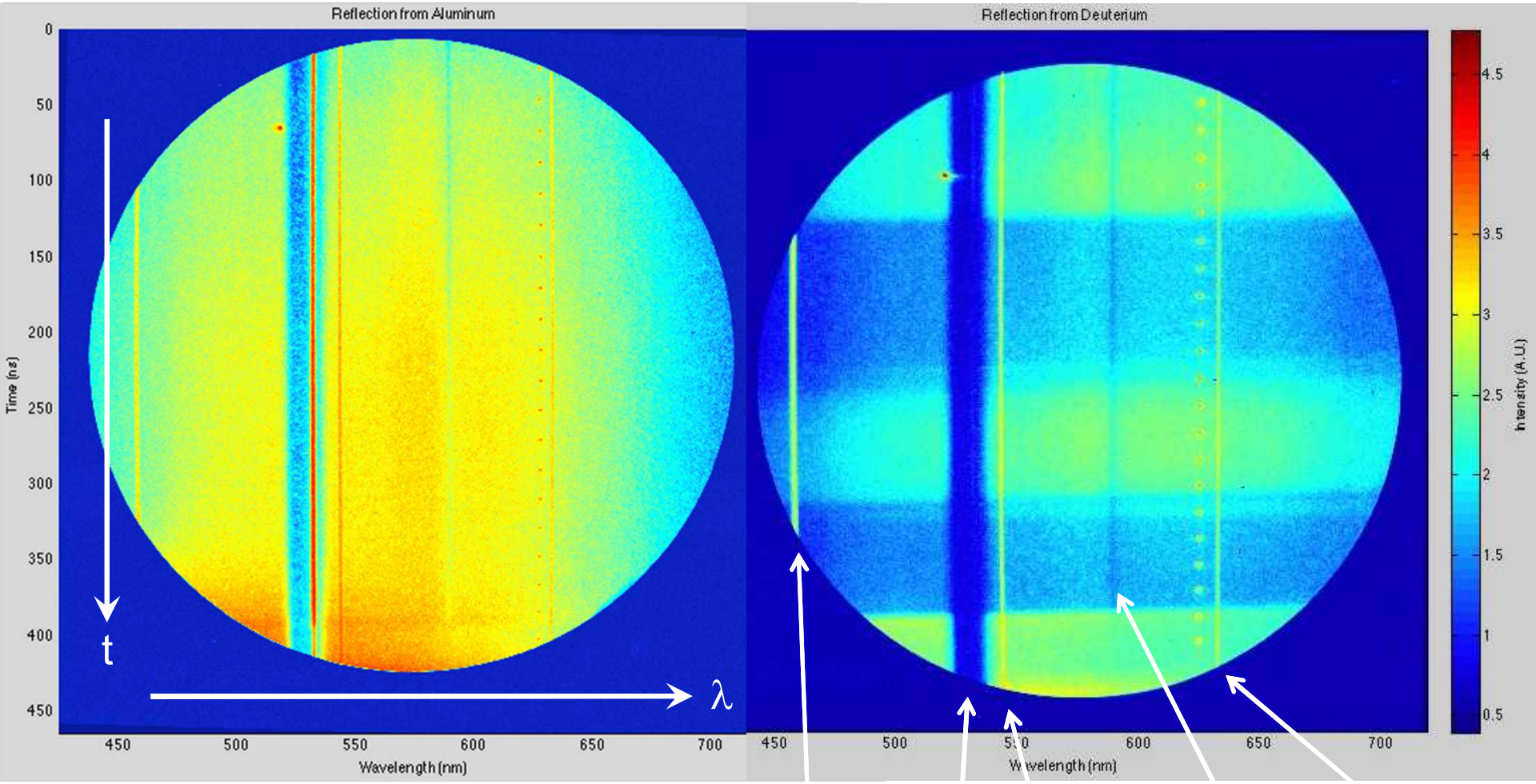
Stripline experimental profiles



SVS system provides data to infer reflectivity

Reflection from aluminum coating

Reflection from deuterium



Wavelength range ~450-700 nm

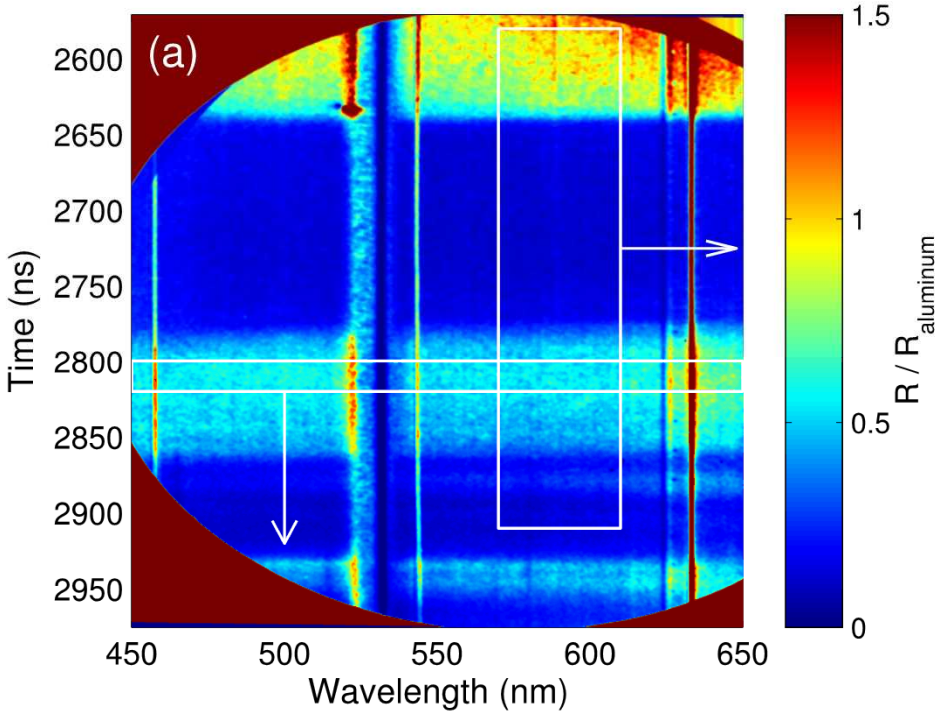
457.9 nm

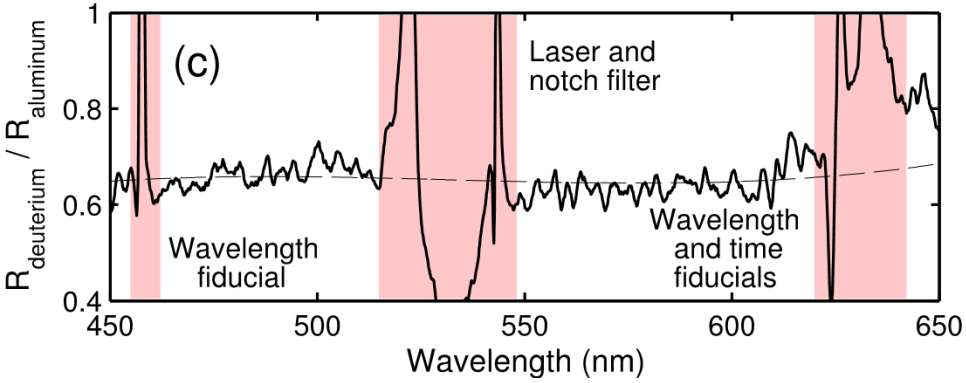
532 / 543.5 nm

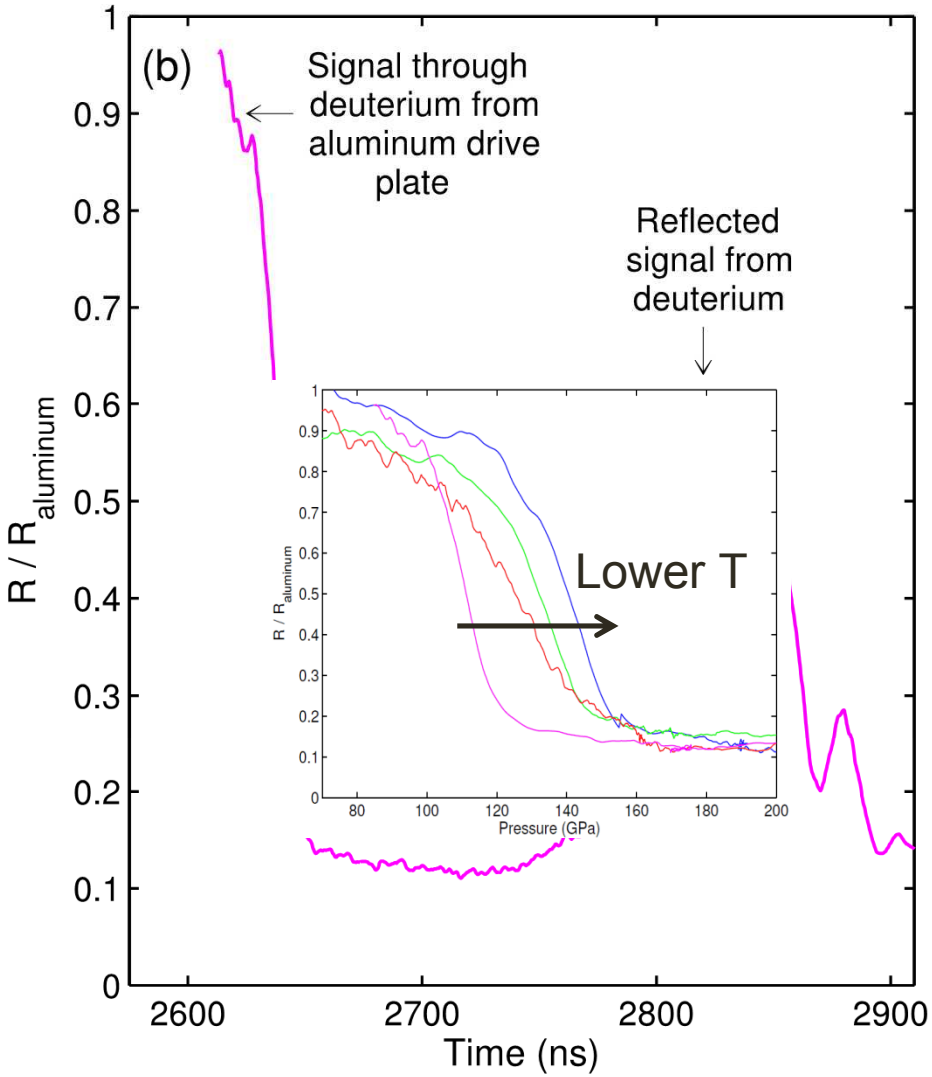
589.3 nm

633 nm

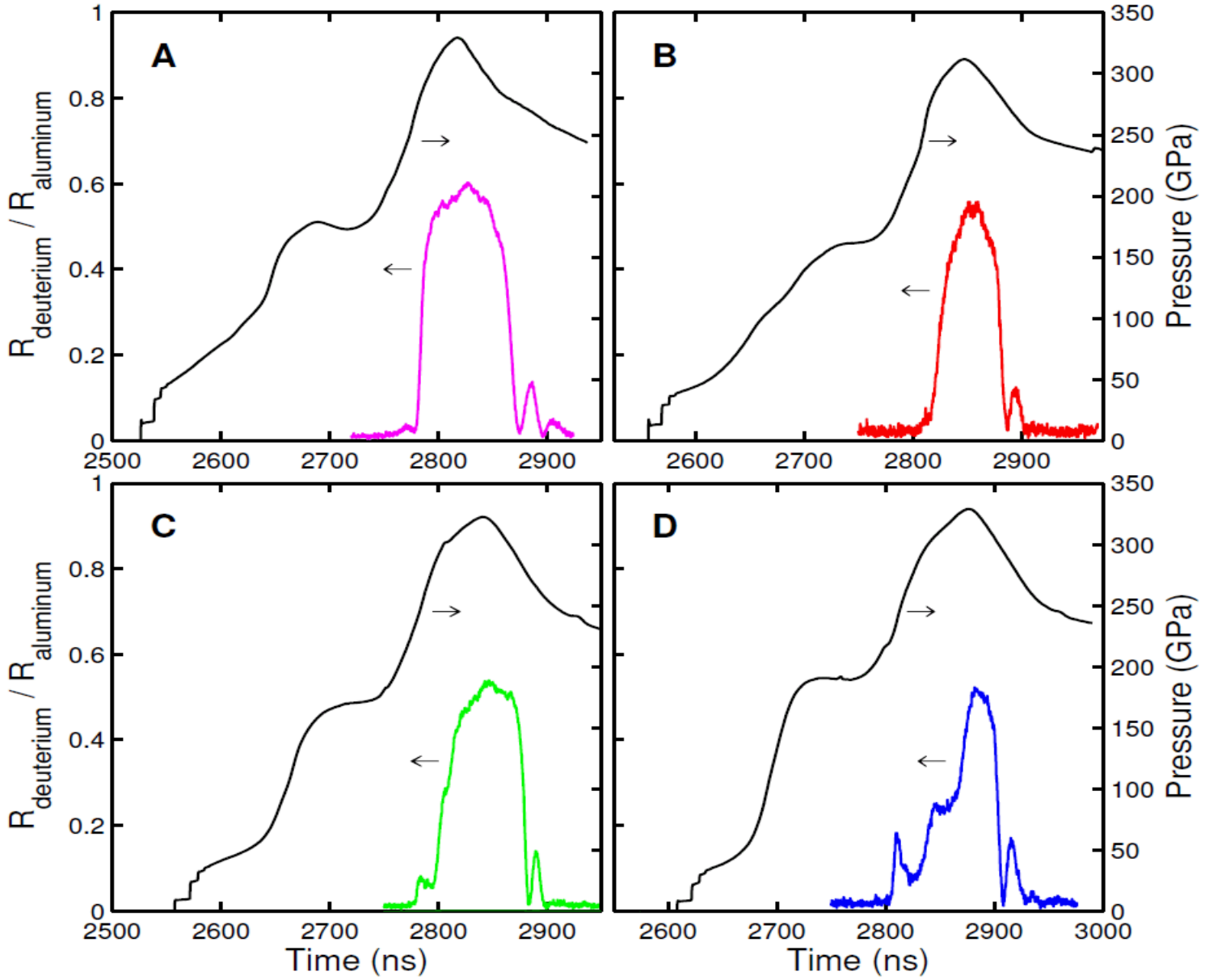
SVS system provides data to infer reflectivity



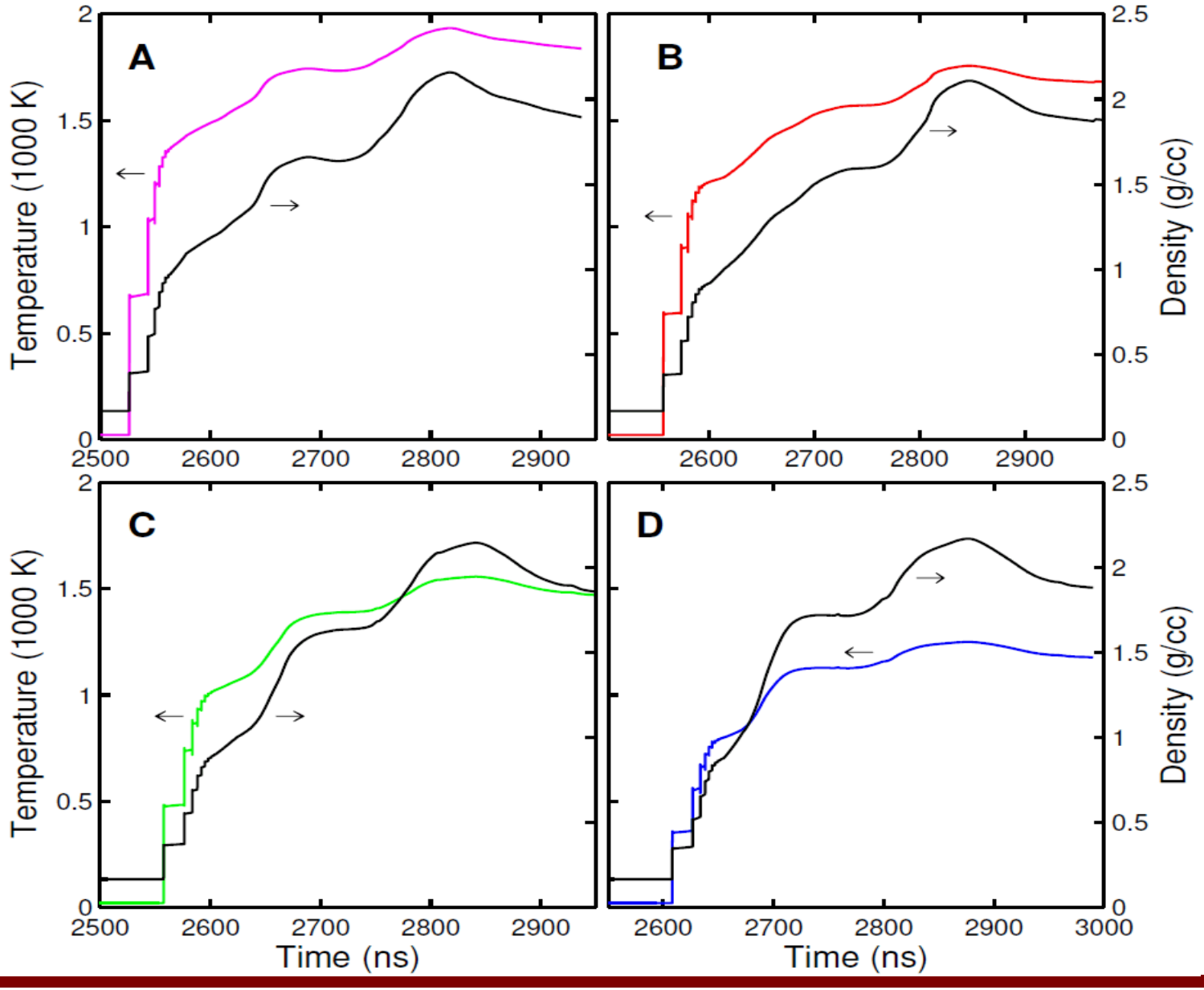




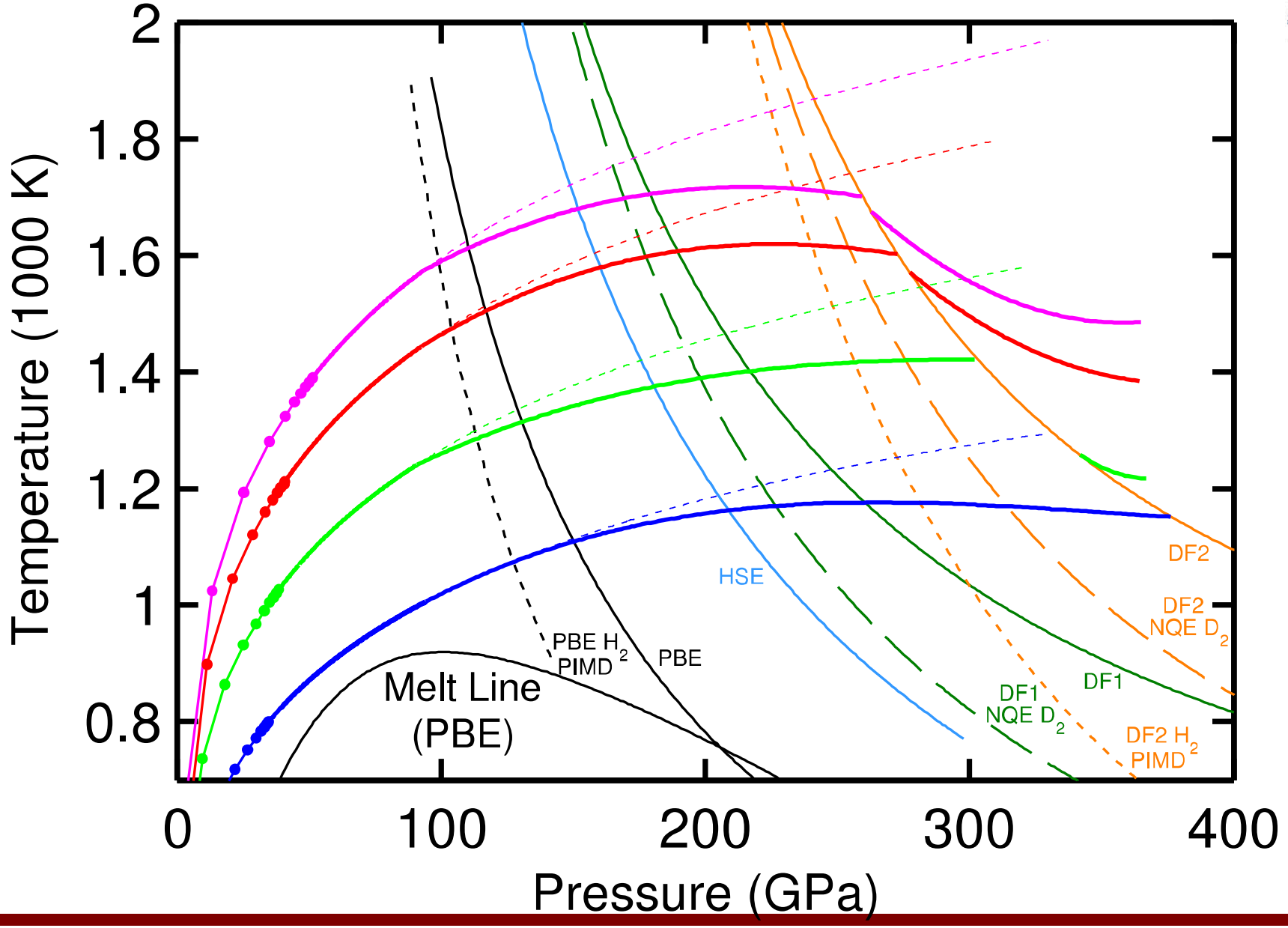
P(t) obtained from v(t) and LiF EOS



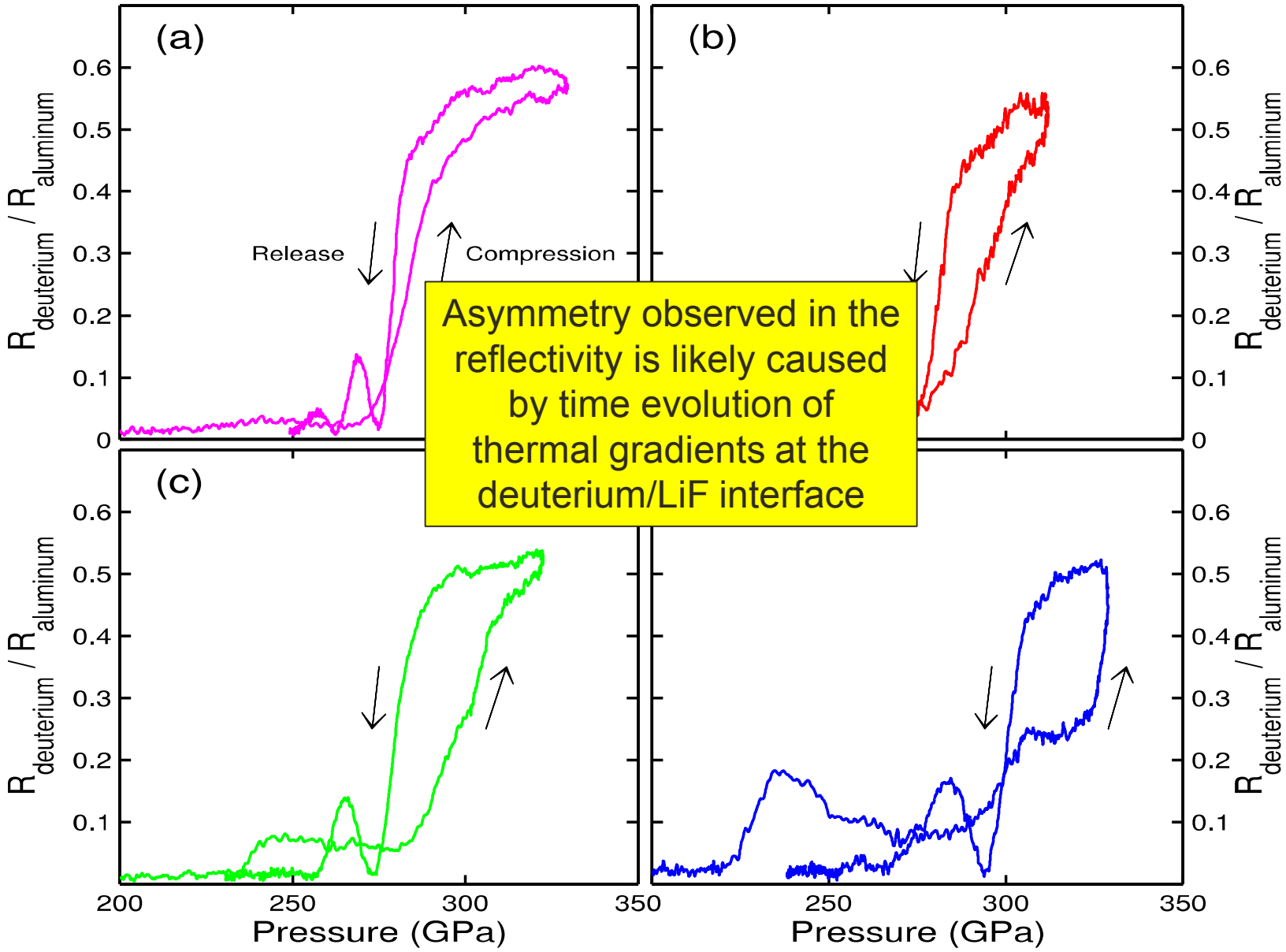
T(t) and ρ(t) obtained from D_2 EOS (Kerley03)



Experimental PT Paths

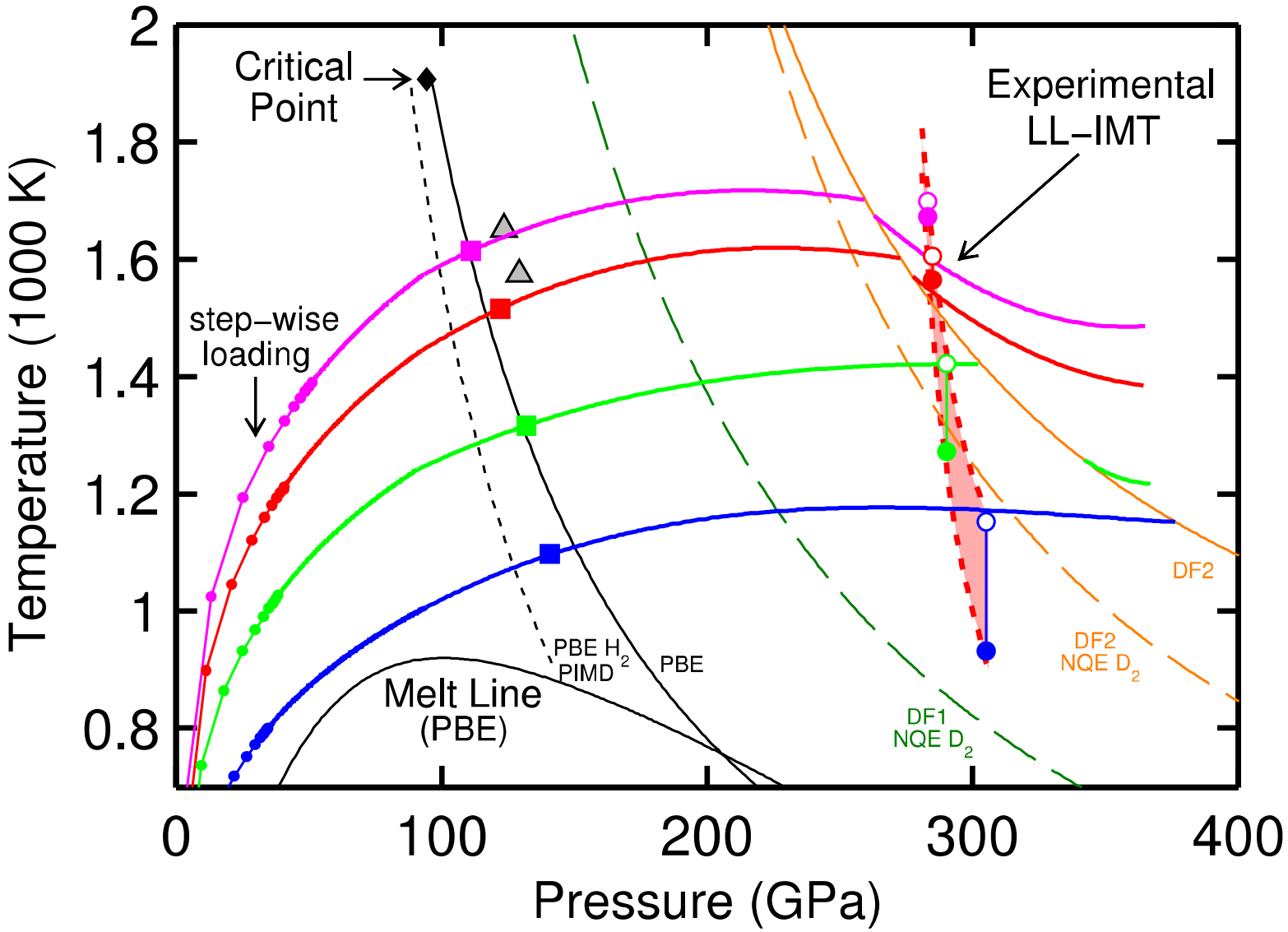


Reflectivity signals mapped to pressure



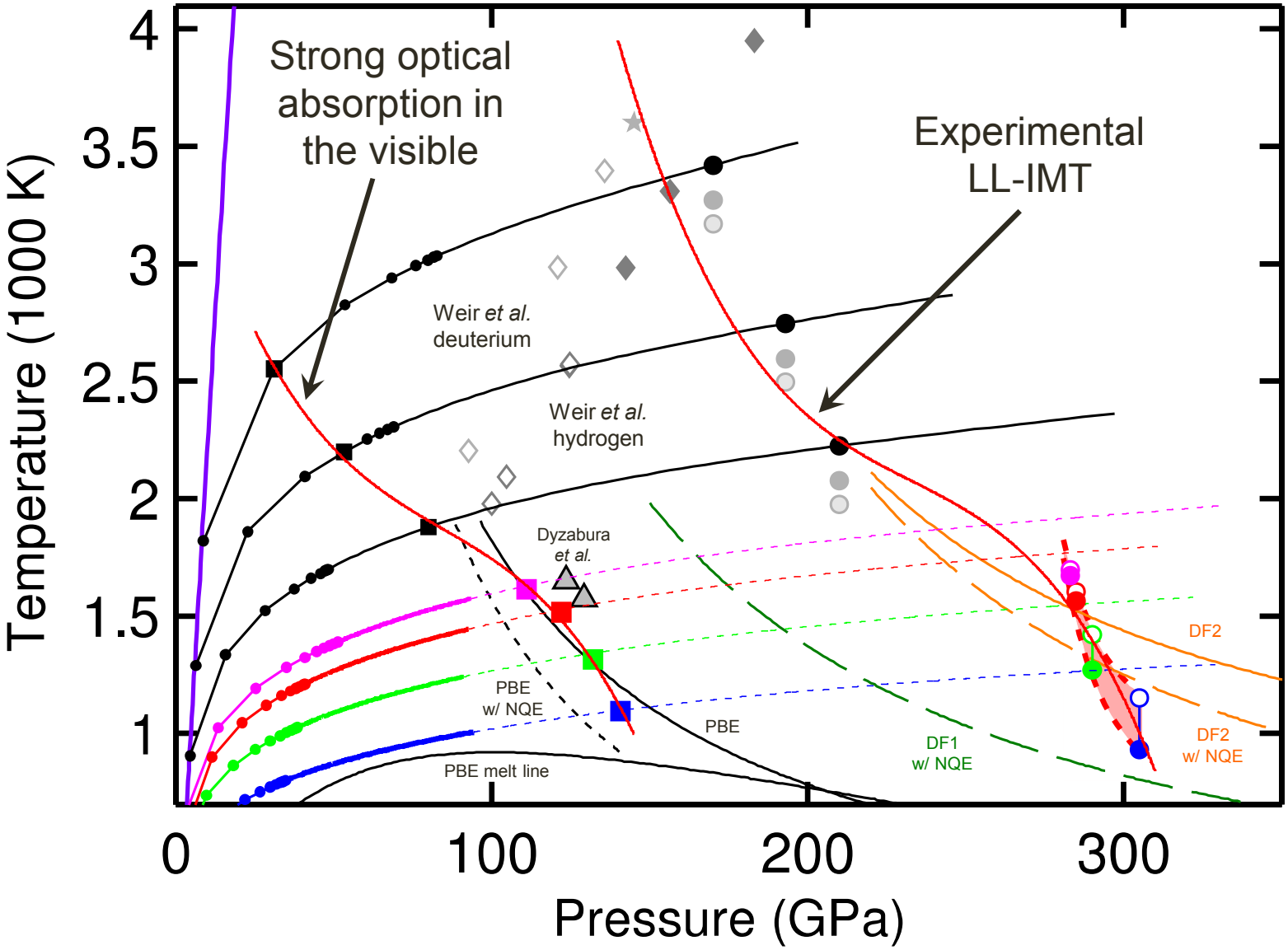
Asymmetry observed in the reflectivity is likely caused by time evolution of thermal gradients at the deuterium/LiF interface

Location of the LL-IMT in deuterium

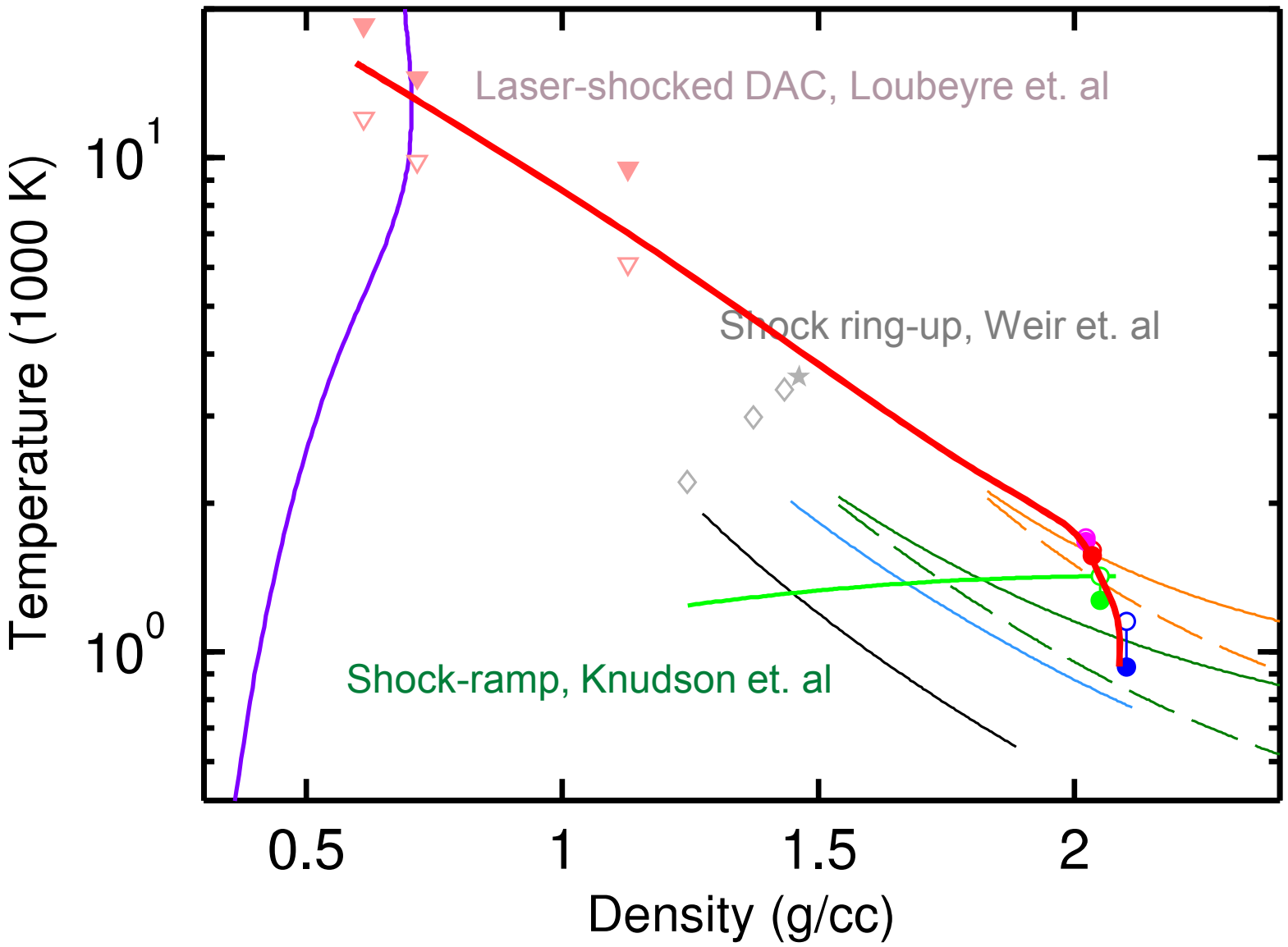


M.D. Knudson et al., Science 348, 1455 (2015)

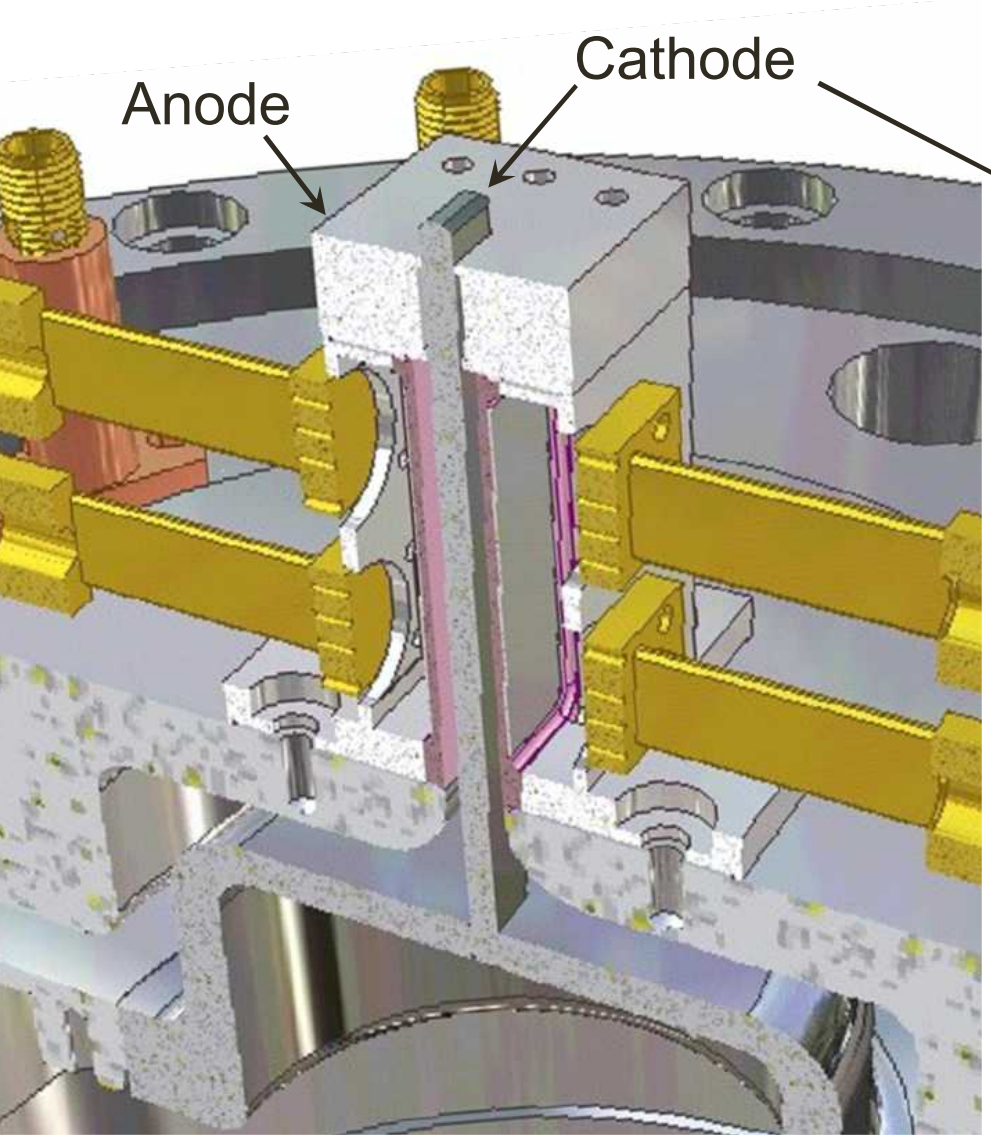
Location of the LL-IMT in deuterium

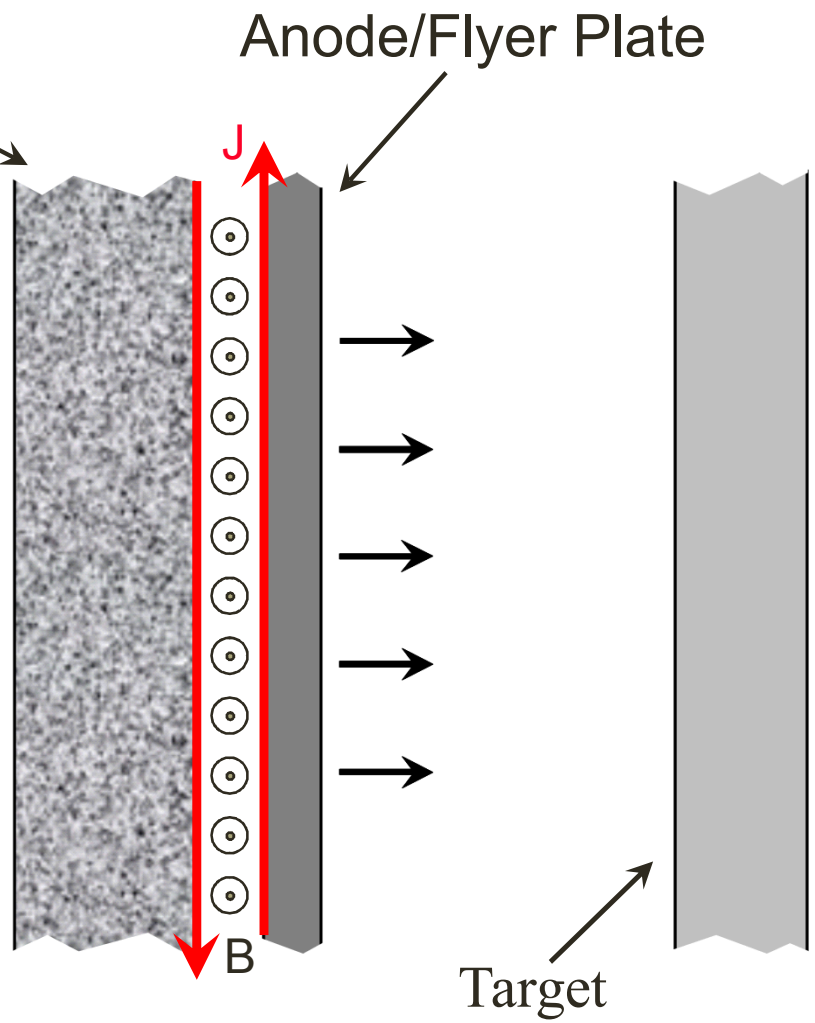


Extended P-ρ diagram for deuterium

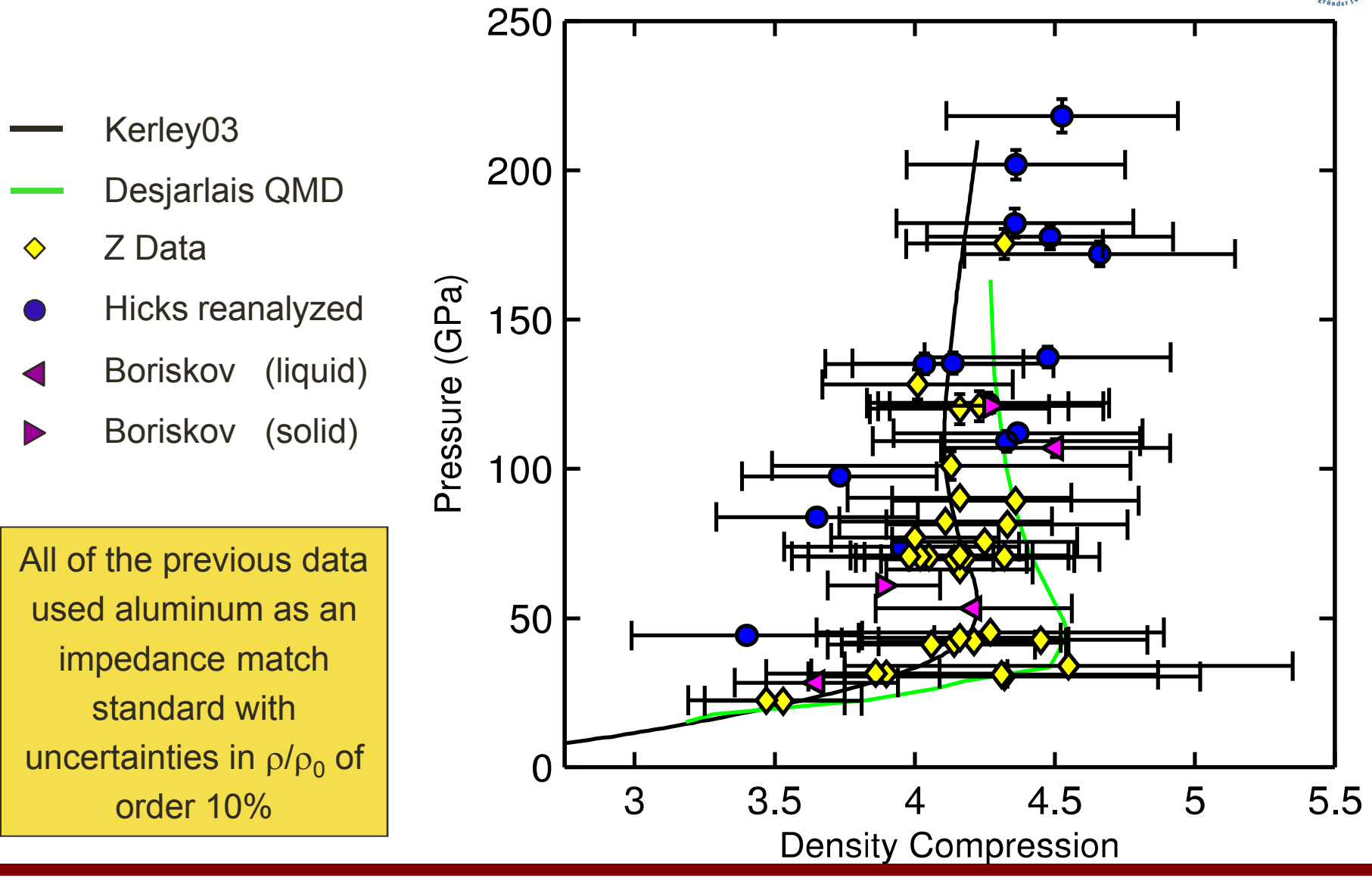


Magnetic pressure can also be used to launch flyer plates to high velocity





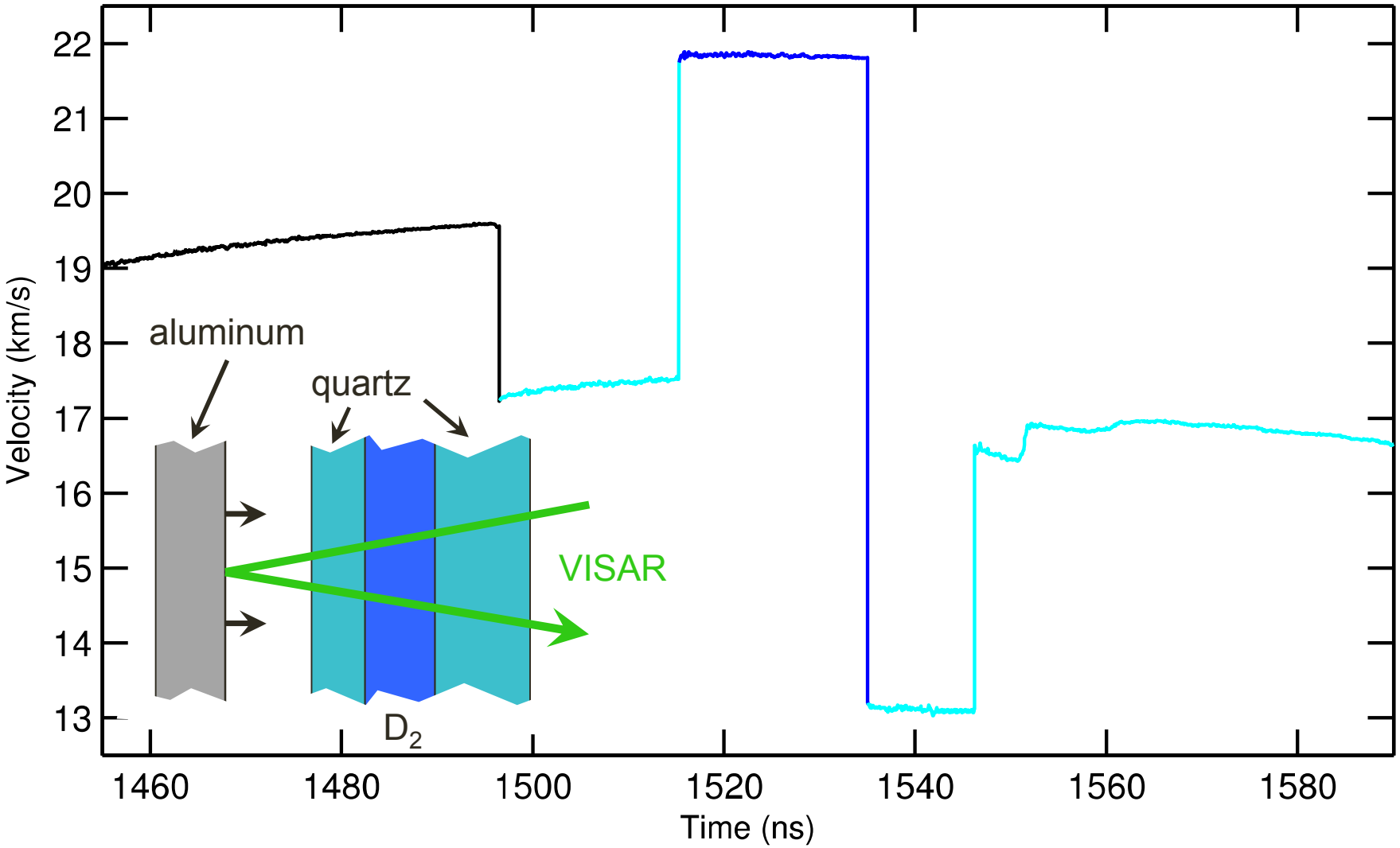
Previous Hugoniot data for deuterium has relatively large uncertainty and scatter



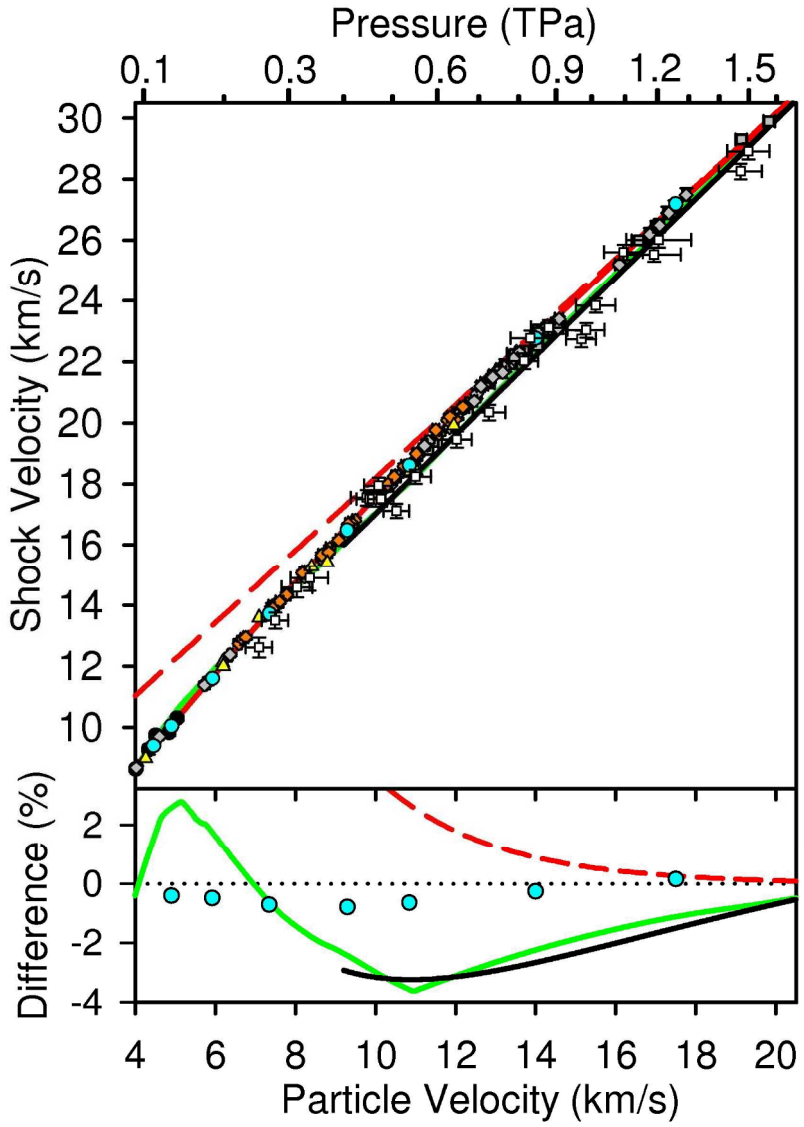
All of the previous data used aluminum as an impedance match standard with uncertainties in ρ/ρ_0 of order 10%

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

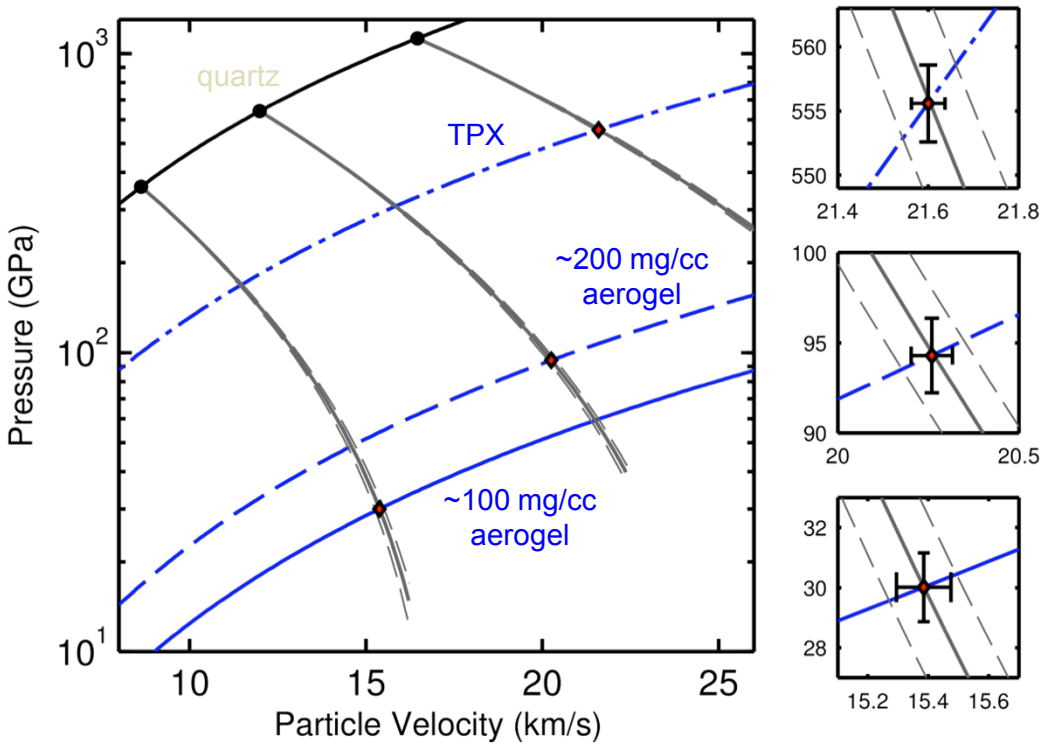
VISAR was used to obtain precise flyer plate and shock velocities in the D_2 and quartz



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

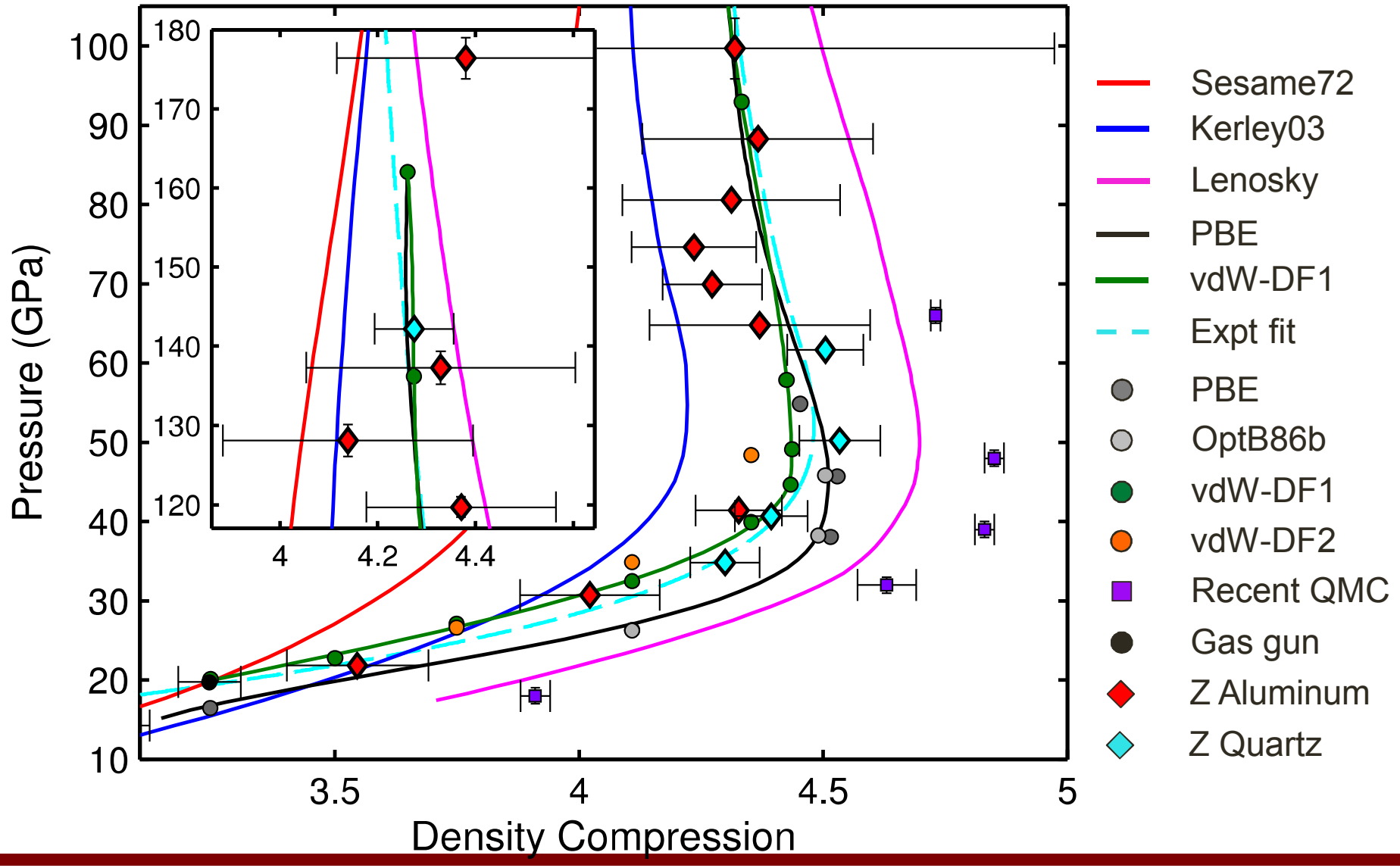


- Nearly 300 Hugoniot points for quartz have been obtained between 1 and 15 Mbar
- A release model was developed using release measurements obtained from TPX, and both ~200 mg/cc and ~100 mg/cc aerogel



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



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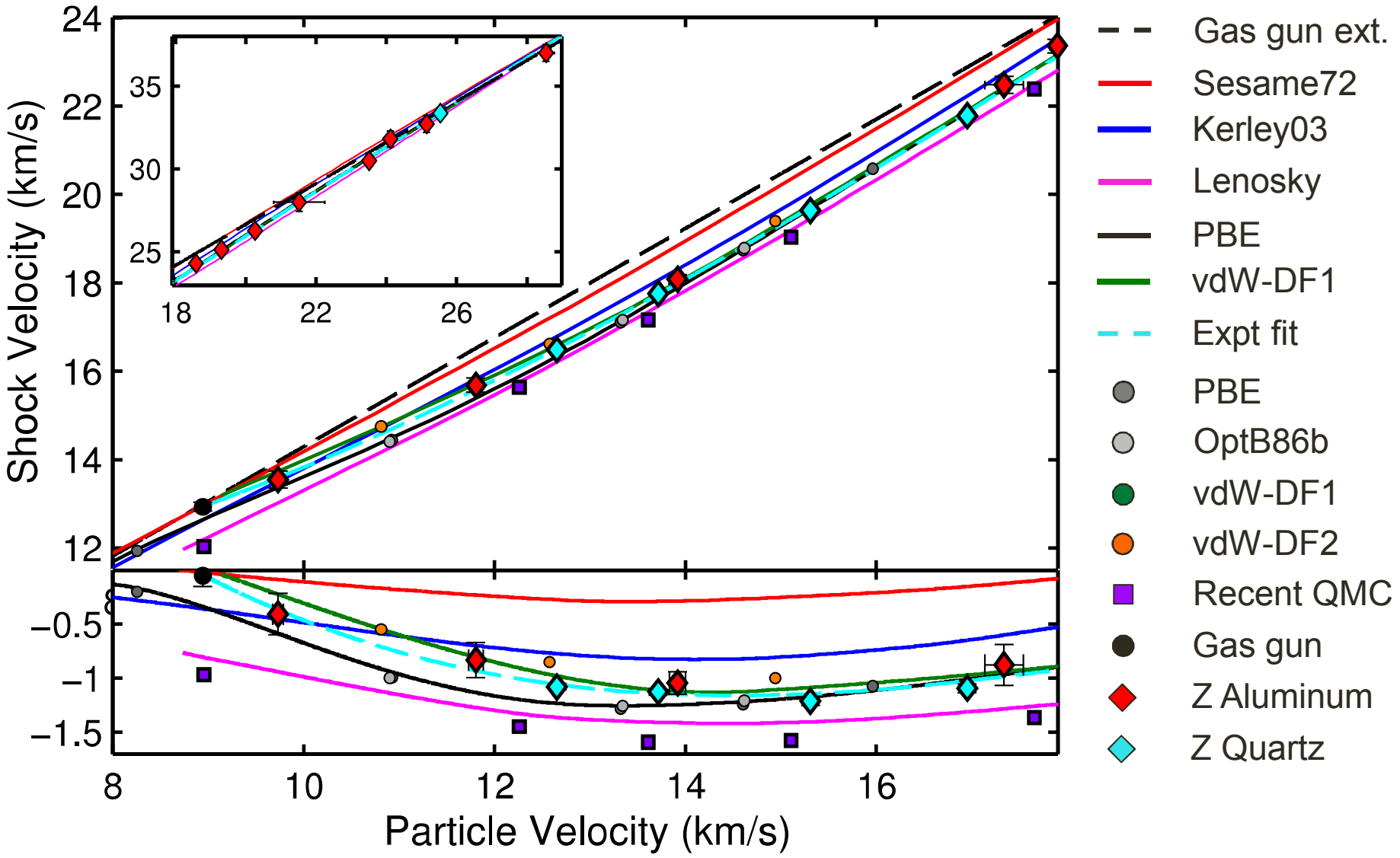
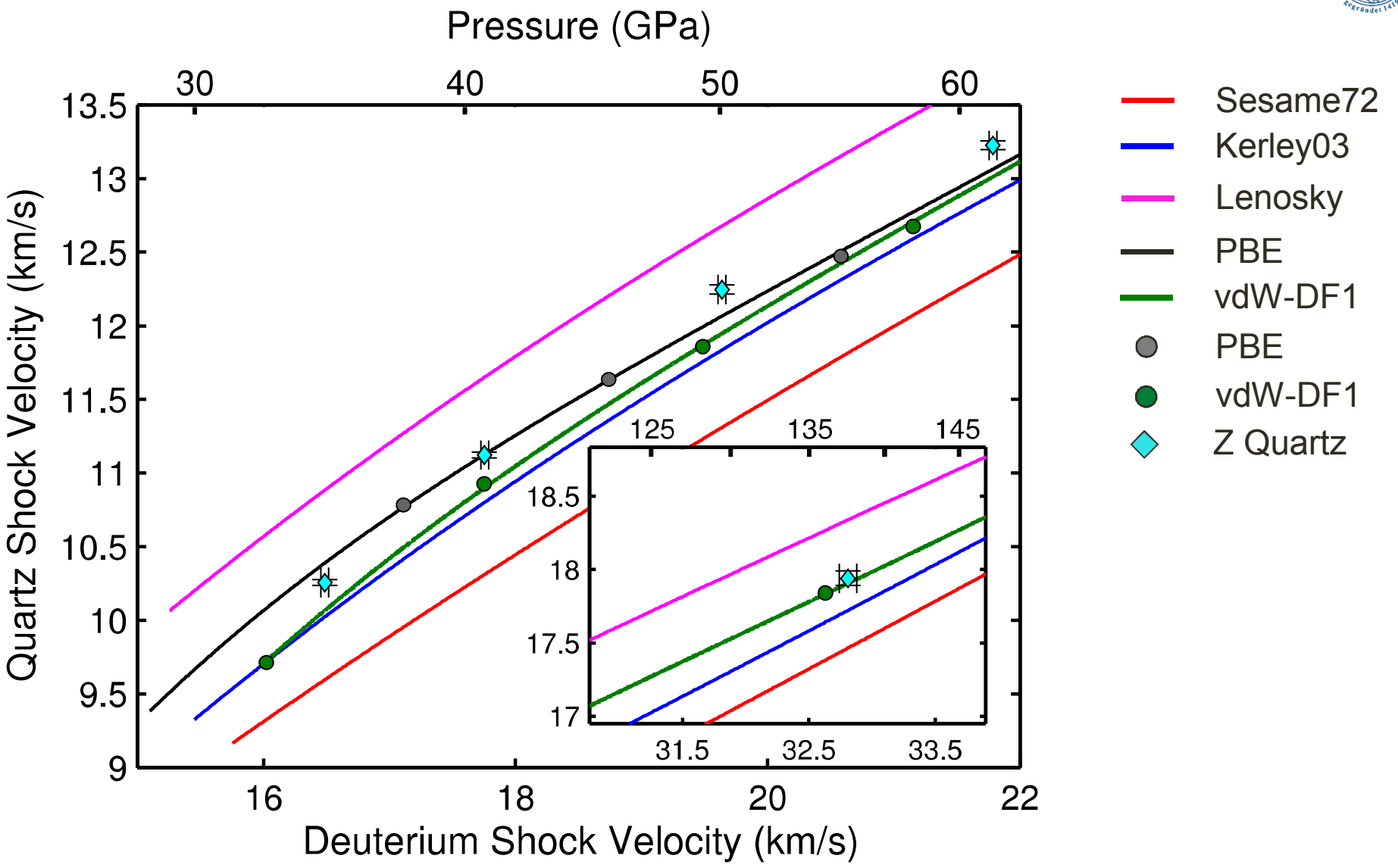


Conclusions from Principal Hugoniot experiments are corroborated by reshock measurements



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
- Metallization at low *T* and along the Hugoniot are in reasonable agreement with non-local vdW functionals

Acknowledgements

Experiment Design/Analysis

Marcus Knudson

Ray Lemke

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Devon Dalton

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Diagnostics

Charlie Meyer

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Jean-Paul Davis

Mark Savage

Ken Struve

Keith LeChien

Brian Stoltzfus

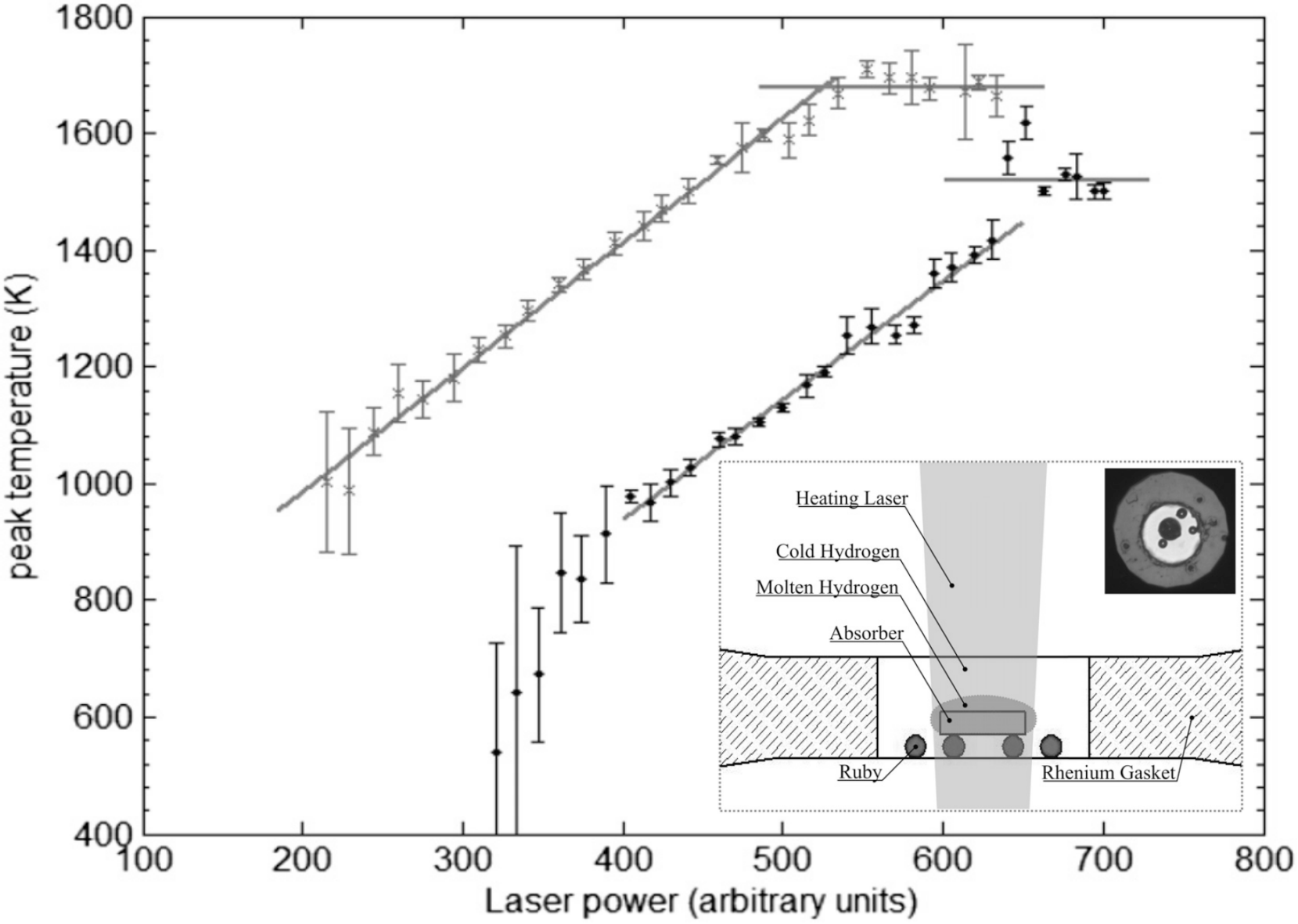
Dave Hinshelwood

Entire Z crew

University of Rostock

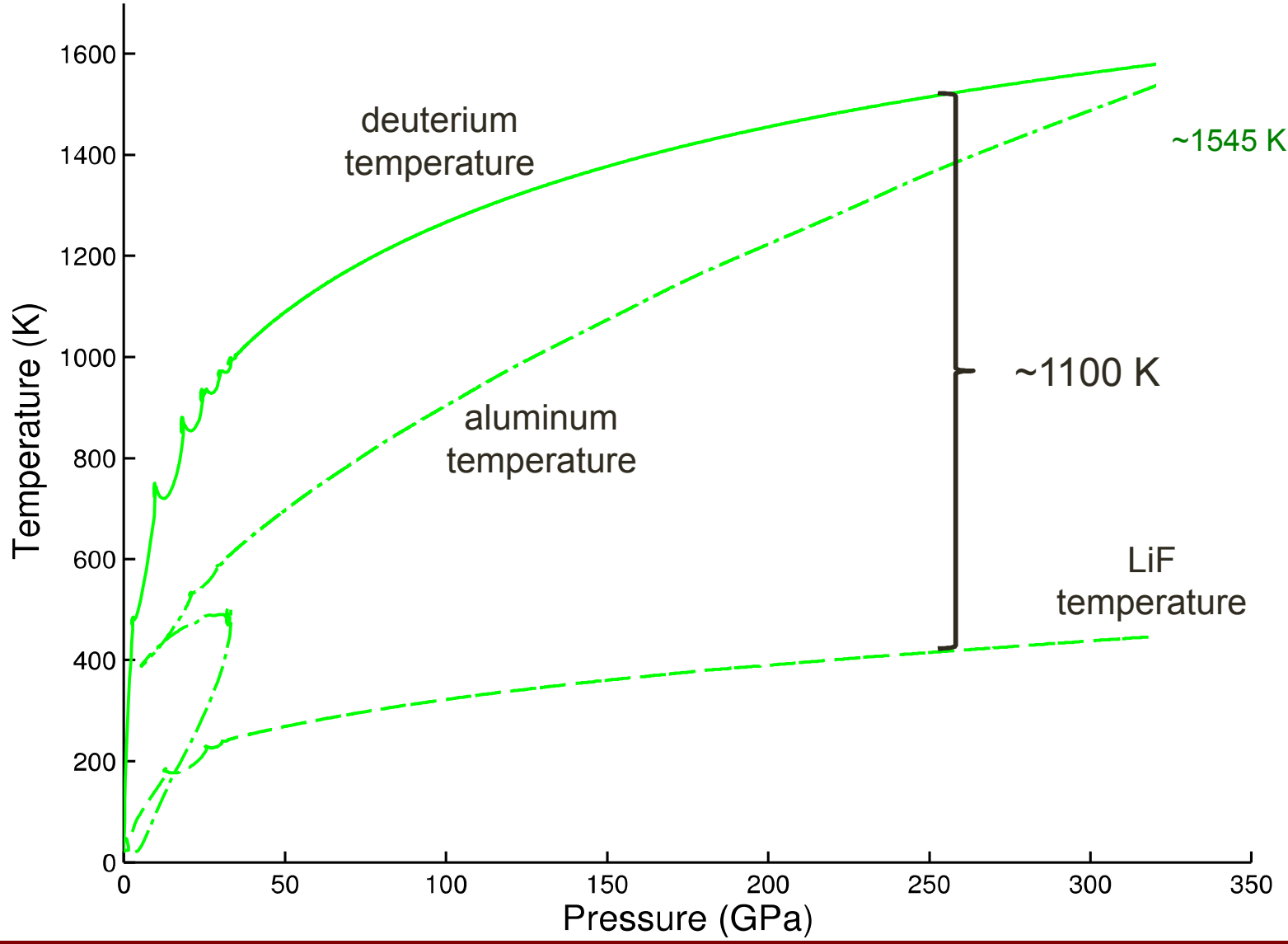
Back-Ups

Dzyabura experiment

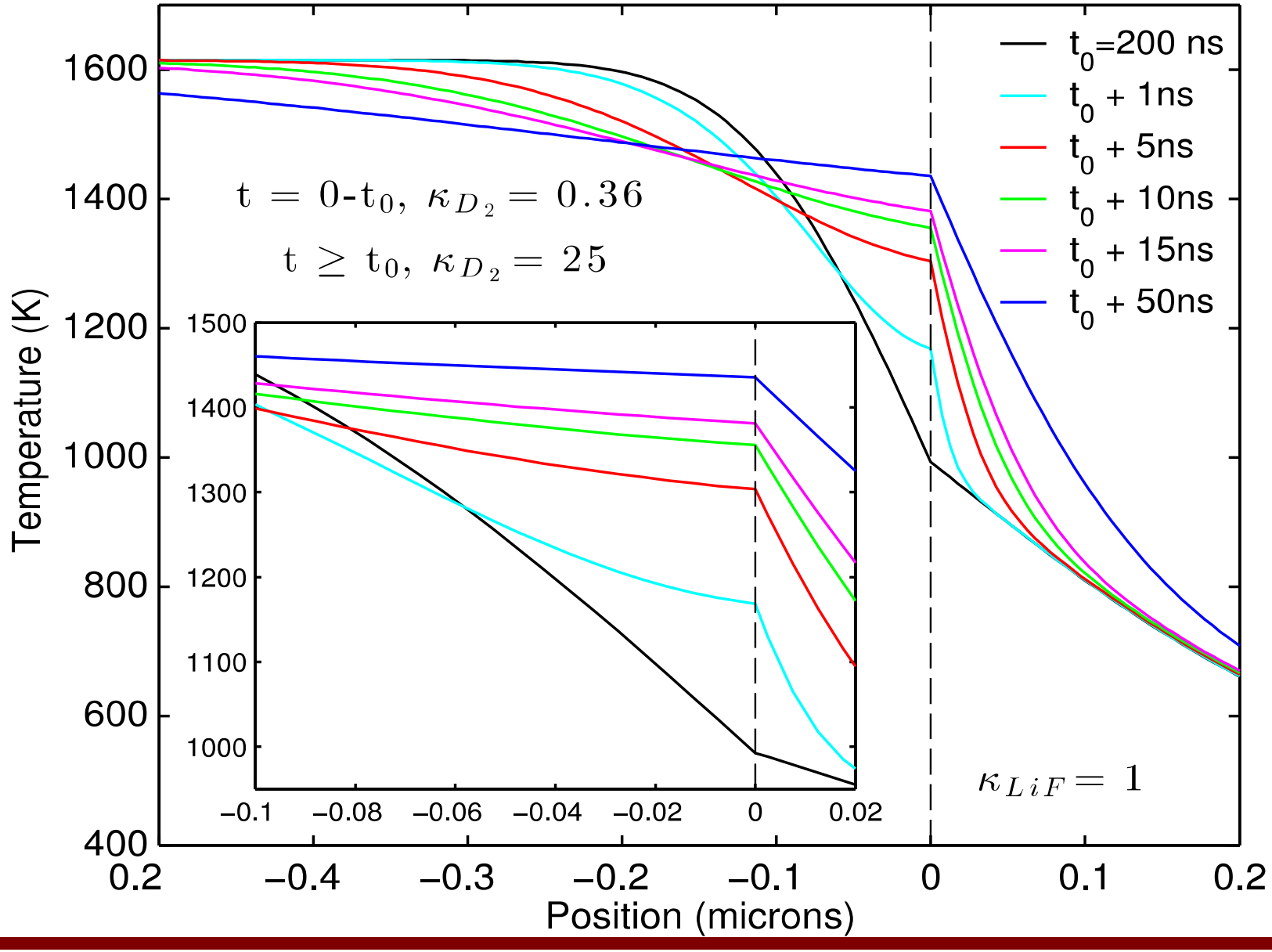


V. Dzyabura, et al. Proc. Natl. Acad. Sci. U.S.A. 110, 8040 (2013)

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



Thermal conduction simulations



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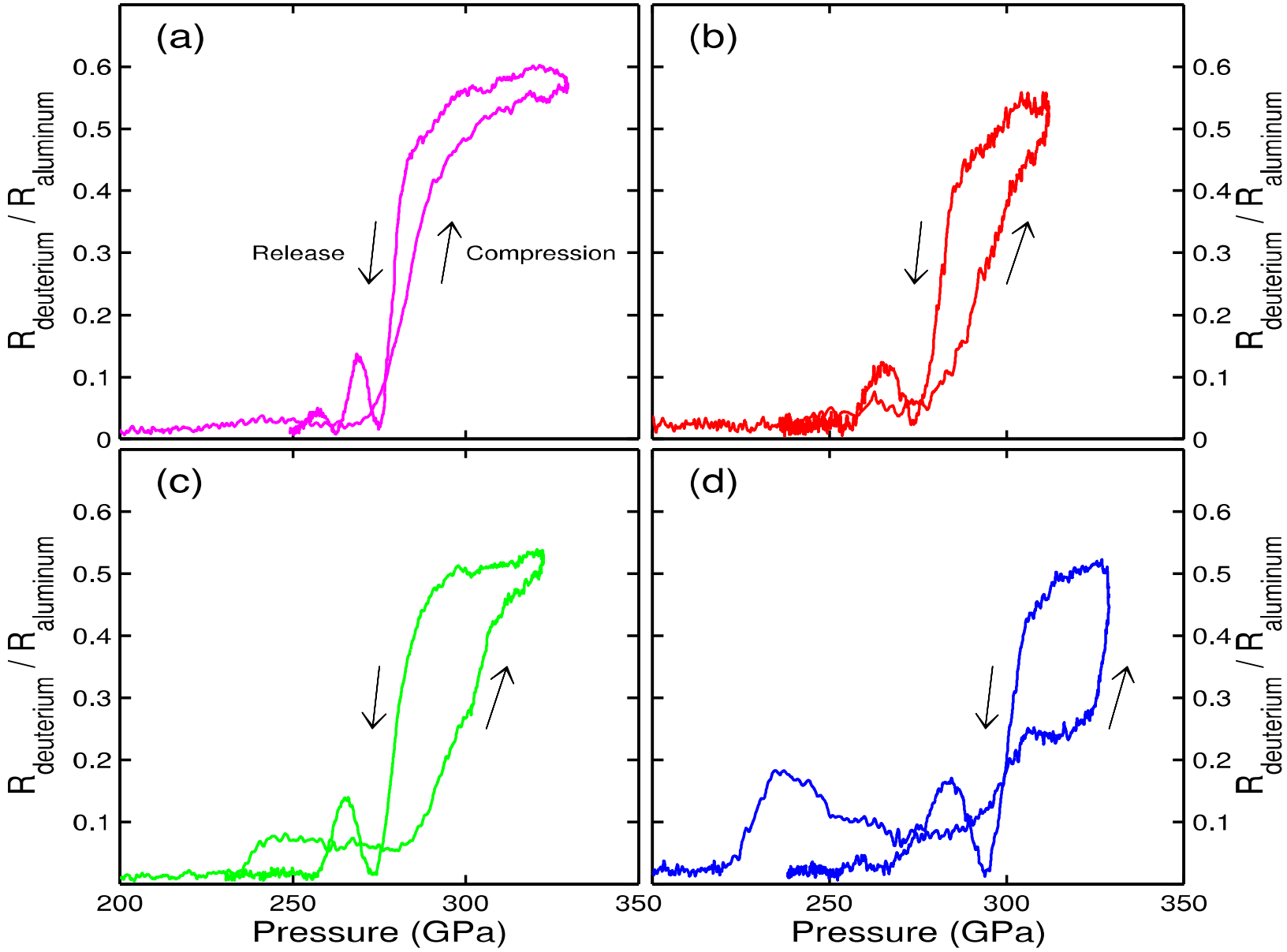
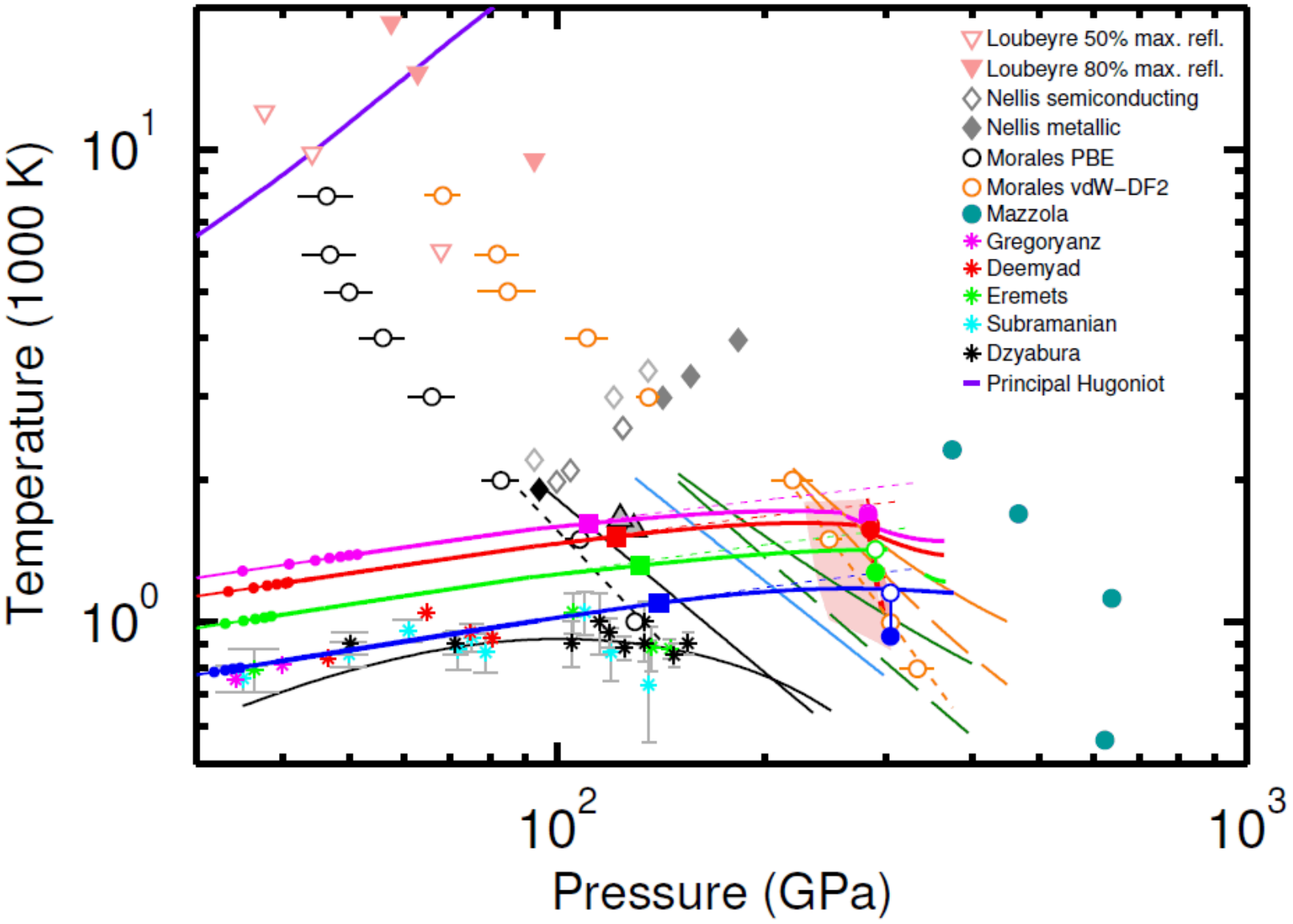
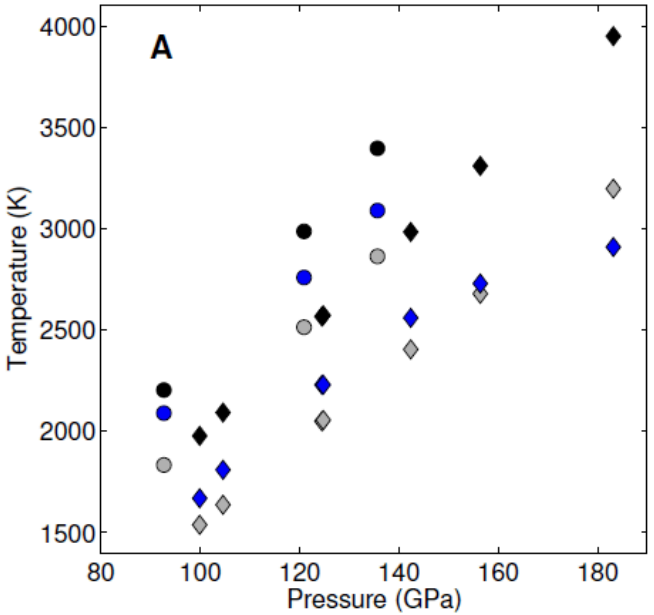
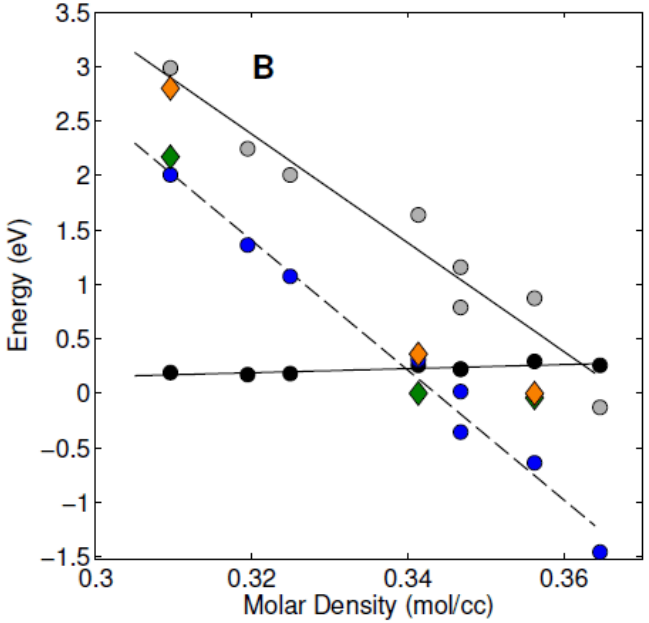


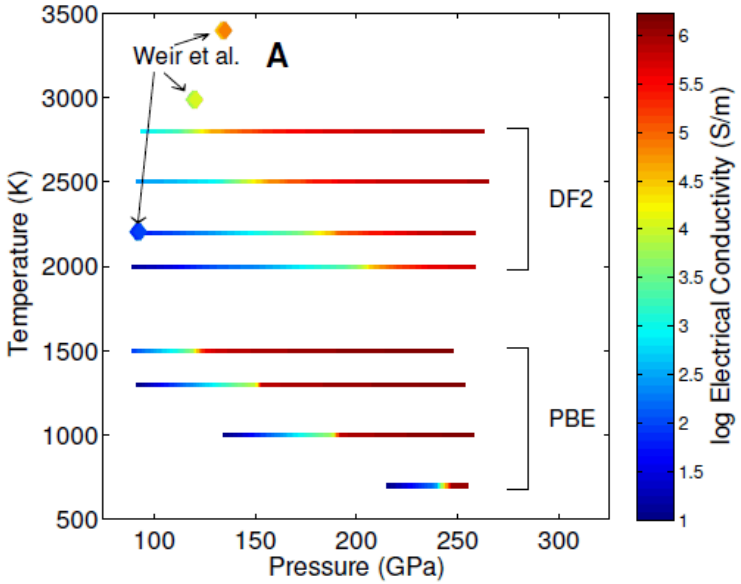
Extended P-T diagram for hydrogen

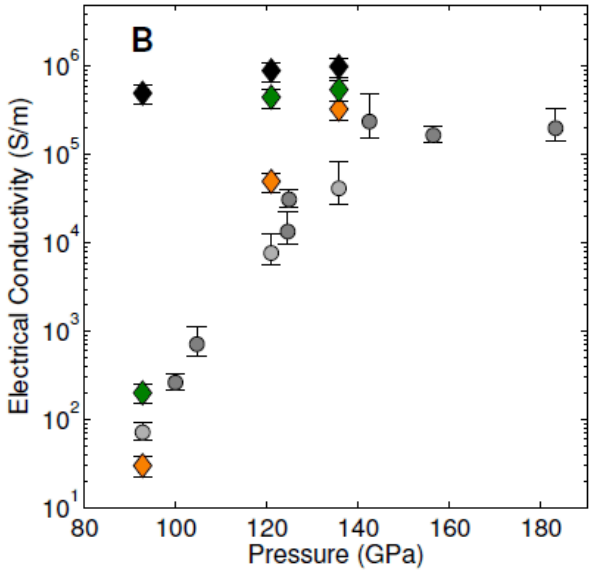


Reanalysis of Weir et al data

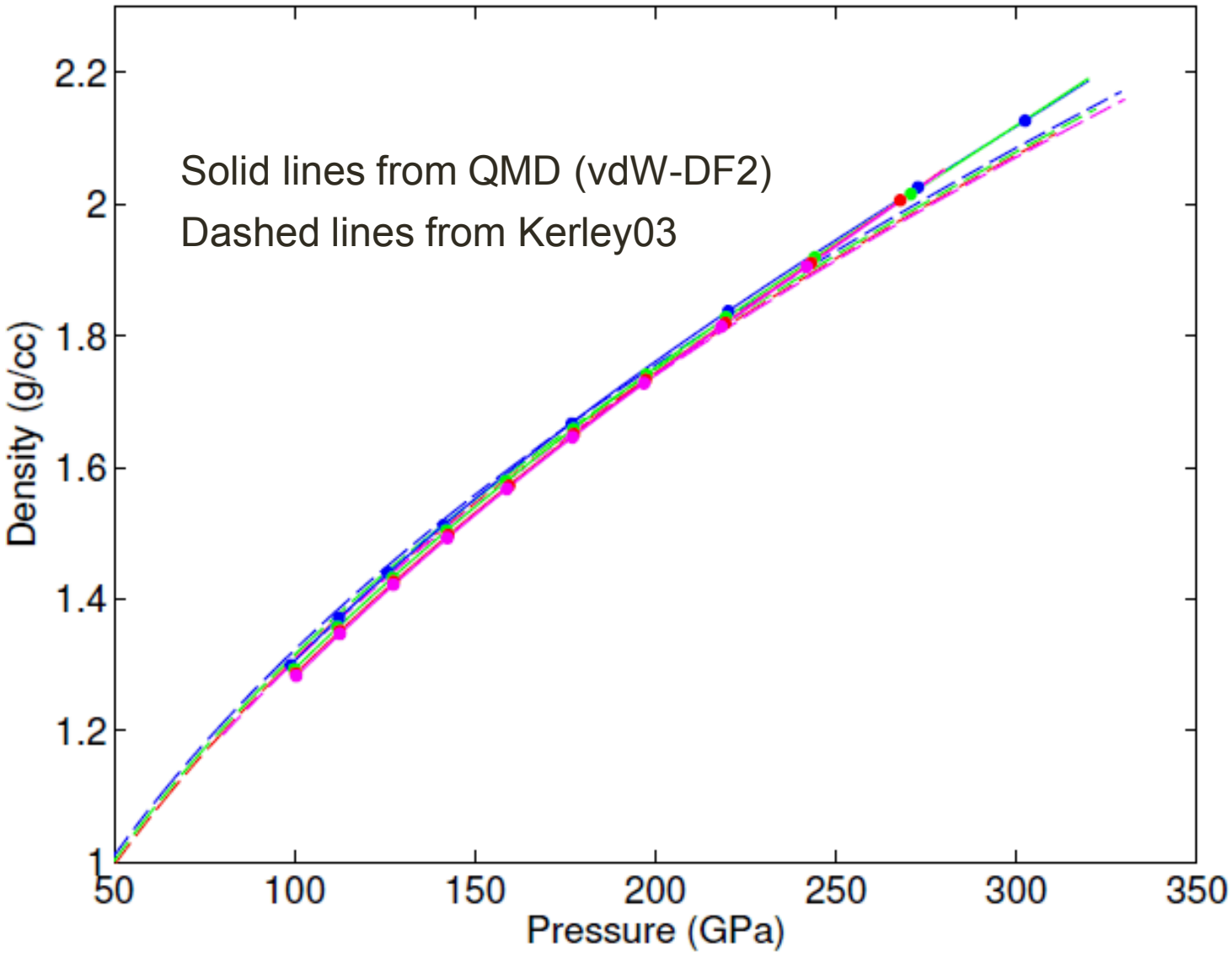






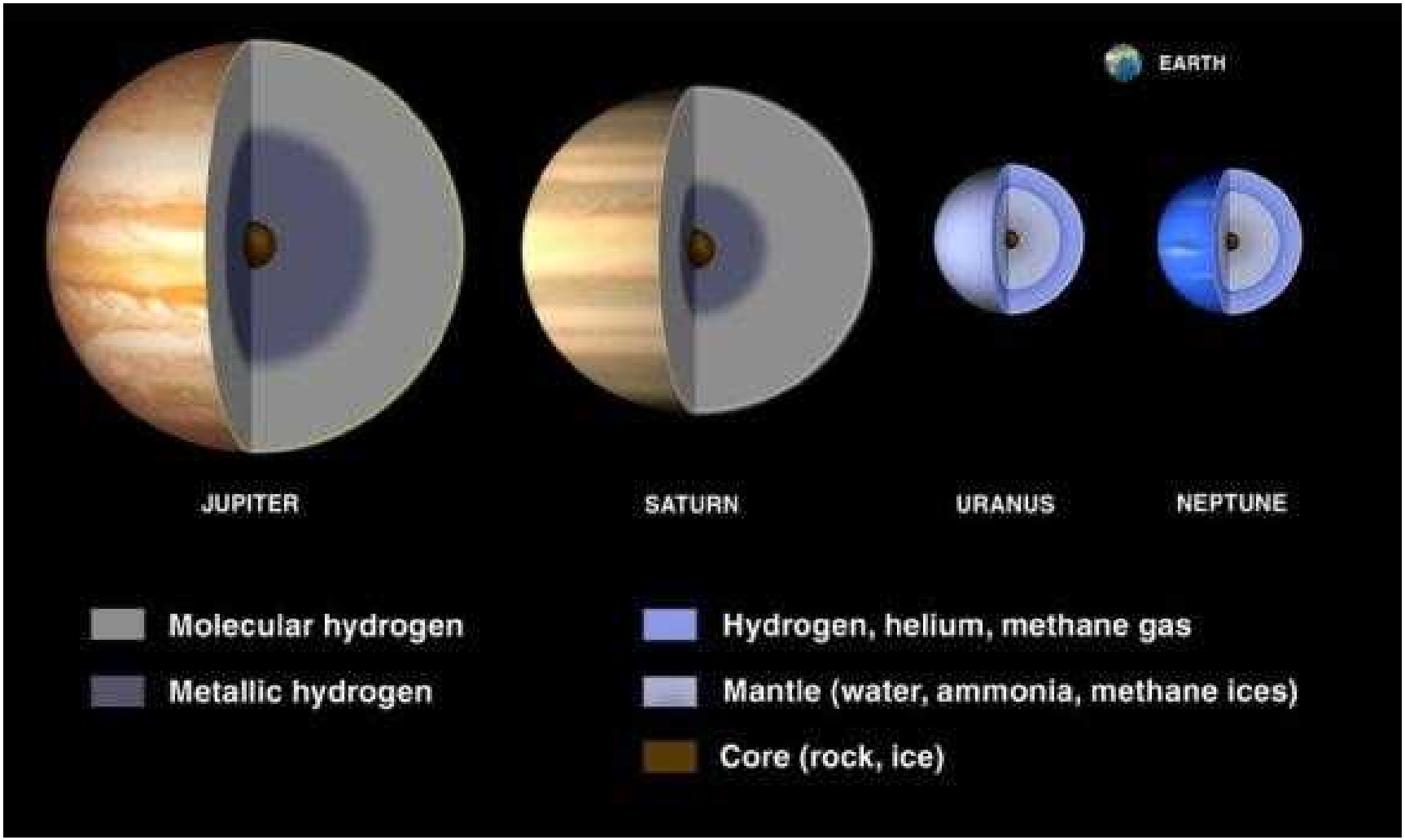


P(ρ) relatively insensitive to EOS model

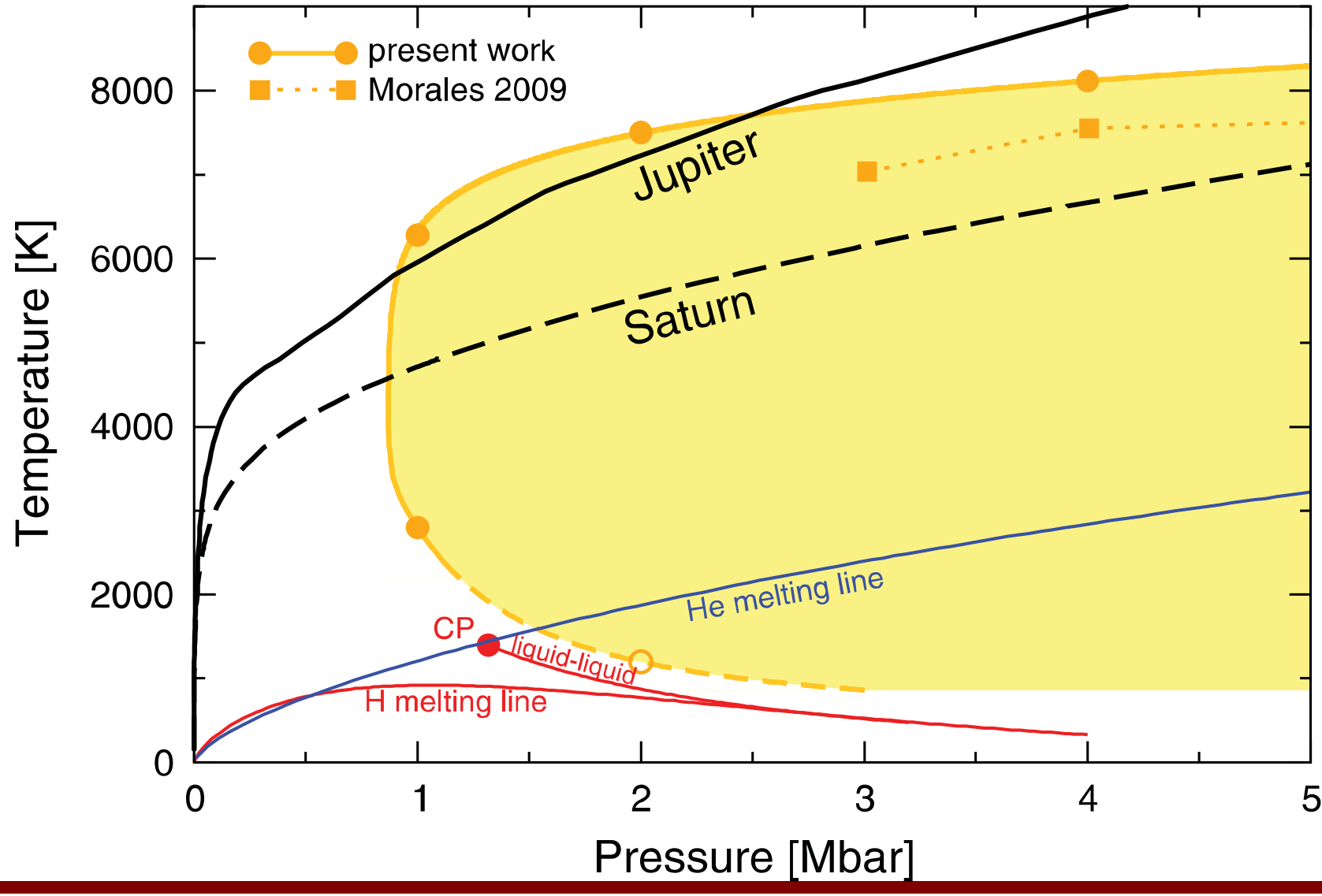


Giant planets in the Solar system

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

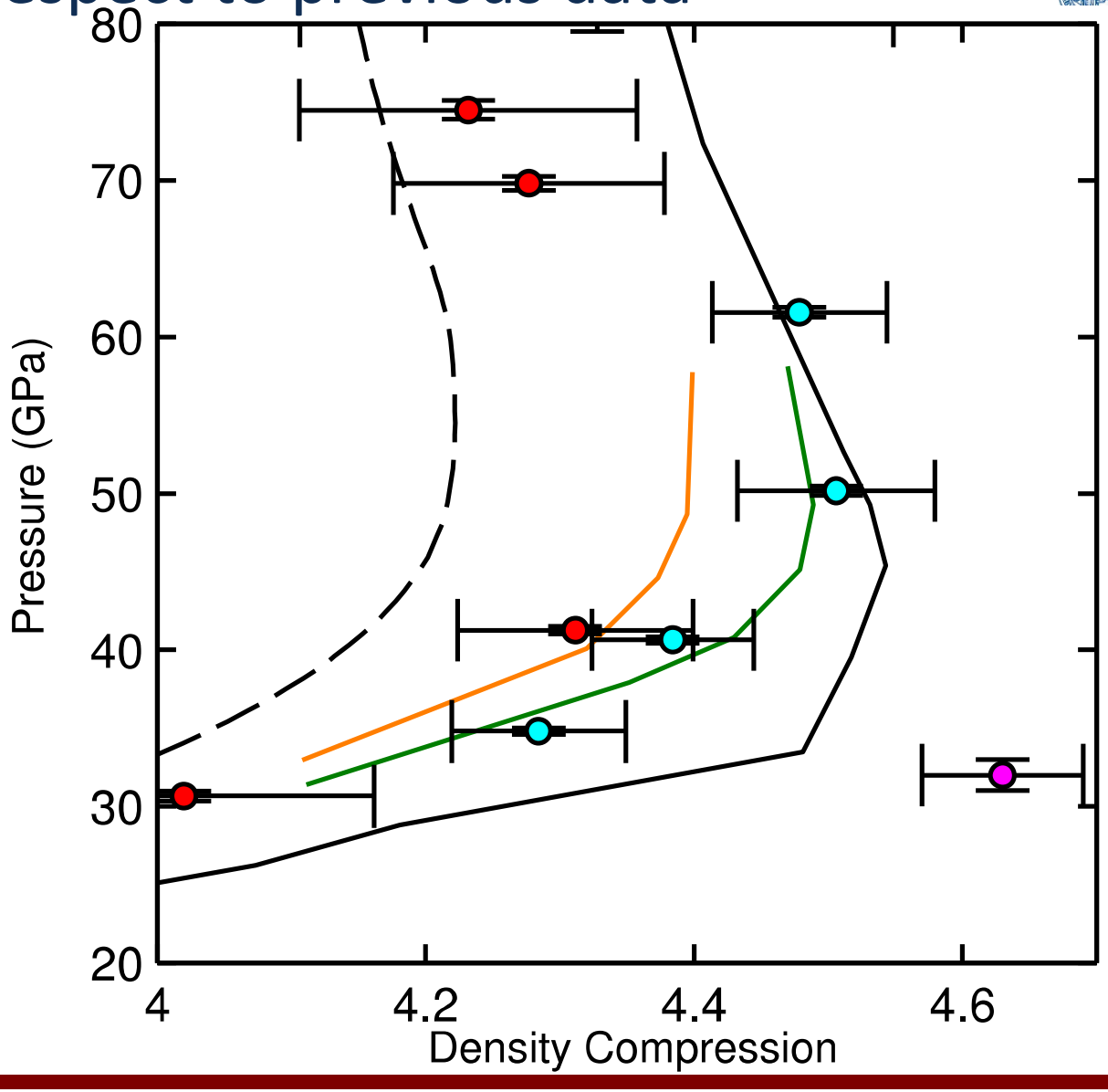
Sandia National Laboratories

UNIVERSITÄT ROSTOCK

- Kerley03
- PBE
- vdW-DF2
- vdW-DF1
- Z Quartz standard
- Z Aluminum standard
- Recent QMC

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)