Phase separation at the dimer-superconductor transition in $Ir_{1-x}Rh_xTe_2$

a tale of a negative result

Emil S. Bozin

Condensed Matter Physics and Materials Science Department
Brookhaven National Laboratory

Physical Review B **98**, 134506 (2018)
Physical Review B **97**, 174515 (2018)

ADD2019
School and Conference on Analysis of Diffraction Data in Real Space
EPN campus, Grenoble, 17-22 March 2019

March 21, 2019

BROOKHAVEN NATIONAL LABORATORY

Phase separation at the dimer-superconductor transition in $Ir_{1-x}Rh_xTe_2$

R. Yu [α], S. Banerjee [α], H. C. Lei [α], A. M. M. Abeykoon [α], C. Petrovic [α], Z. Guguchia [α], R. Sinclair [β], H. D. Zhou [β]

[α] Condensed Matter Physics and Materials Science Department
Brookhaven National Laboratory

[β] Department of Physics and Astronomy
University of Tennessee

Phase separation at the dimer-superconductor transition in $Ir_{1-x}Rh_xTe_2$

ACKNOWLEDGMENTS:

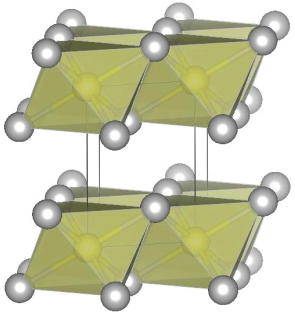
X-ray powder diffraction at 28-ID-2 (XPD) beamline, NSLS II, BNL

Work at BNL supported by DOE-BES DE-SC00112704
Work at UT supported by NSF-DMR-1350002

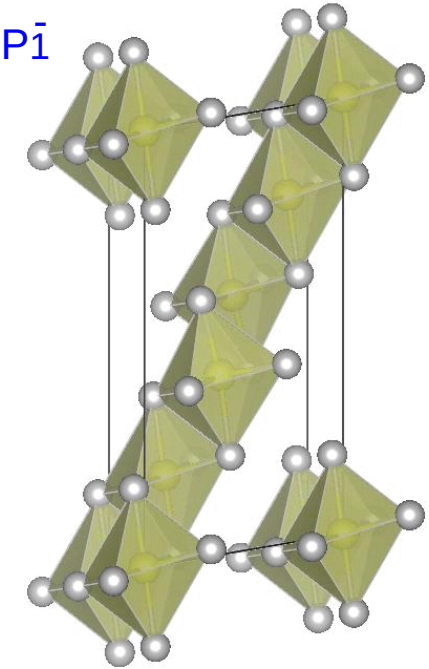
$IrTe_2$: properties

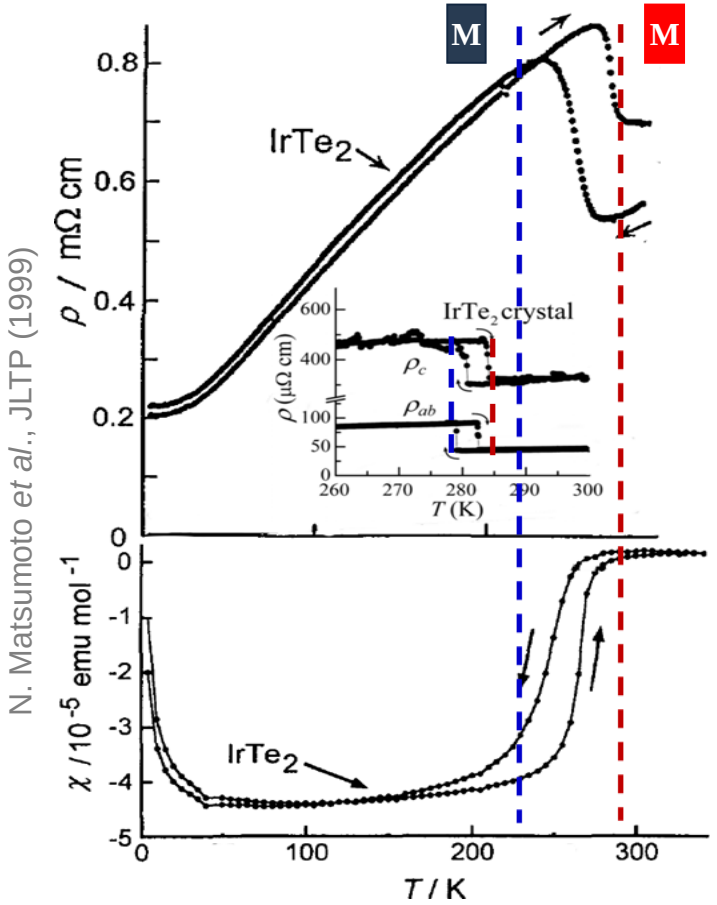
- **HT structure** trigonal $P\bar{3}m1$
- Interlayer spacing smaller than the van der Waals gap
- $Ir^{3+}Te_2^{1.5-}$-like, covalent Te-Te
- Pauli paramagnetic metallic

$P\bar{3}m1$



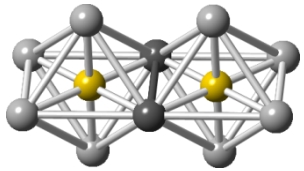
$P\bar{1}$

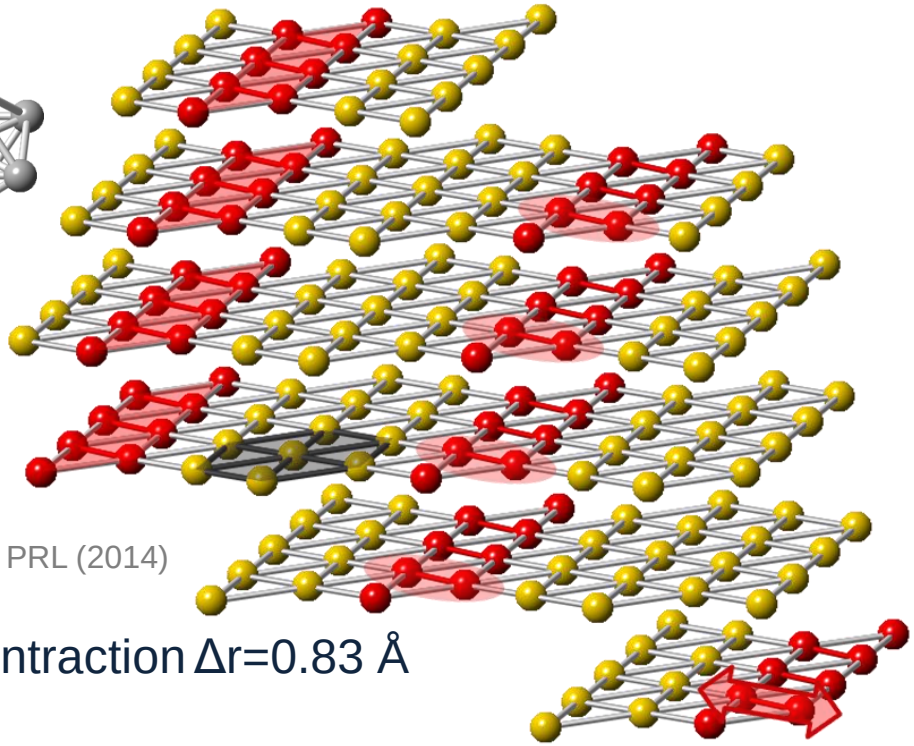




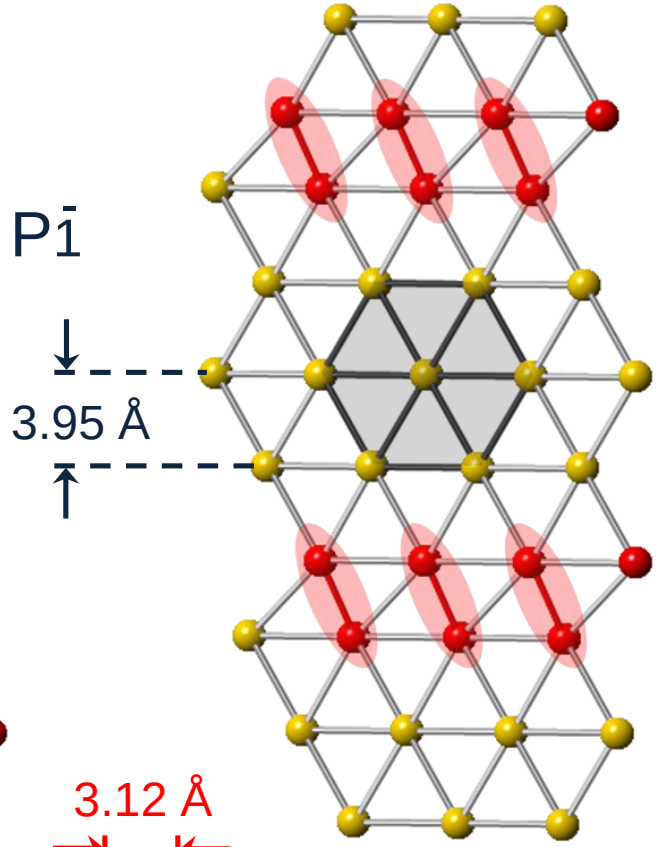
N. Matsumoto *et al.*, JLTP (1999)

$IrTe_2$: dimerization = large distortions



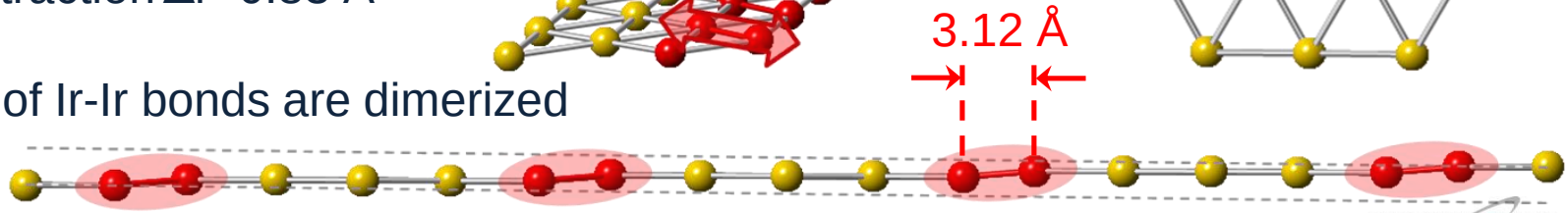


G.L. Pascut *et al.*, PRL (2014)



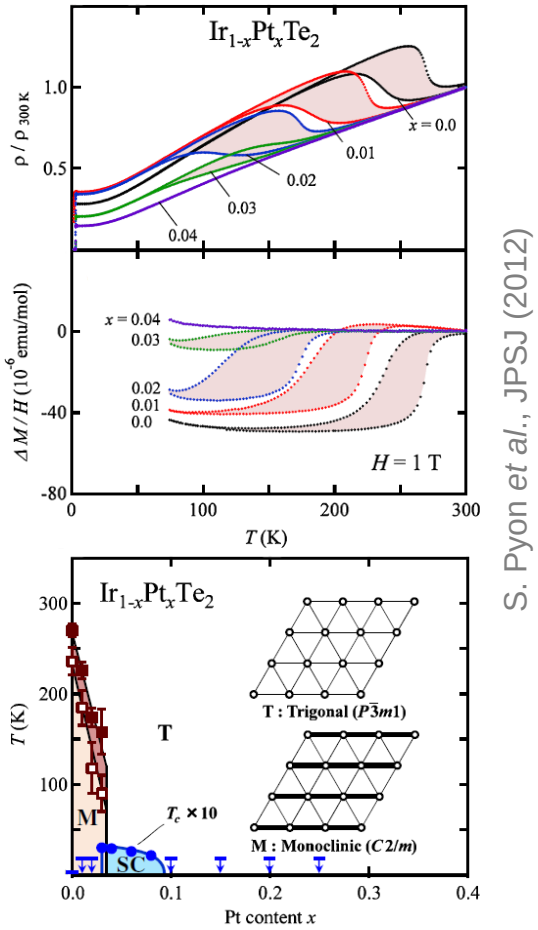
1) Dimer contraction Δr=0.83 Å

2) Only ~6% of Ir-Ir bonds are dimerized

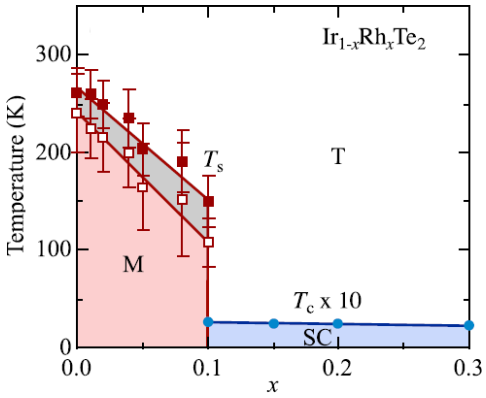


Substitution/intercalation suppresses LT phase and SC appears

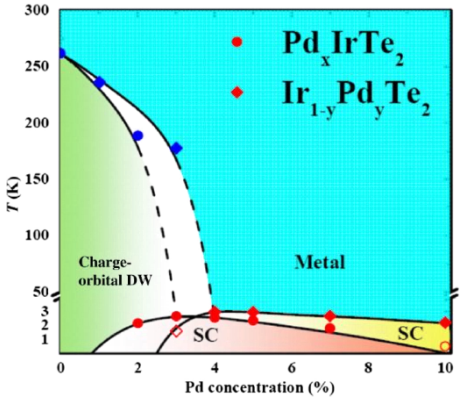
- Reminiscent of unconventional SCs
- Looks like a tunable competition at play



S. Pyon *et al.*, JPSJ (2012)

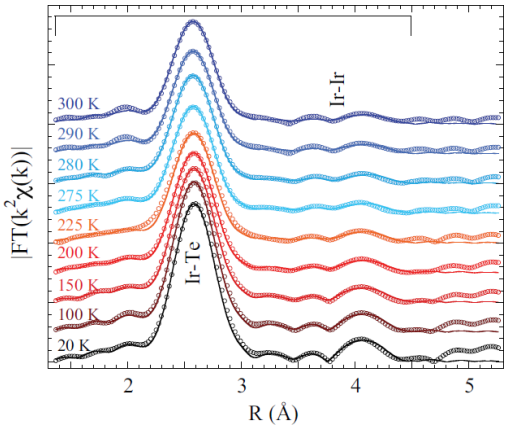


K. Kudo *et al.*, JPSJ (2013)



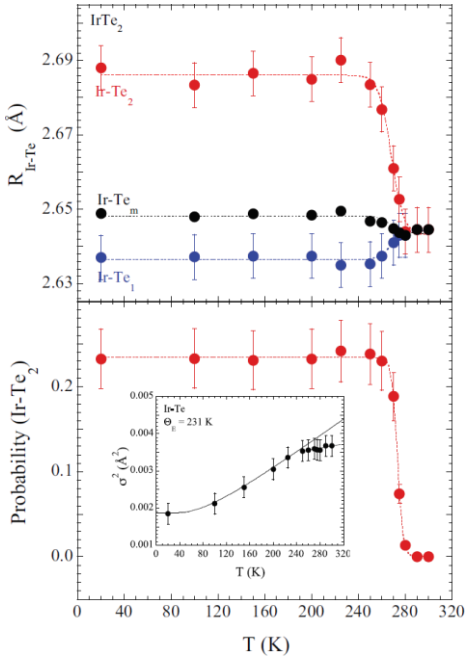
J.J.. Yang *et al.*, PRL (2012)

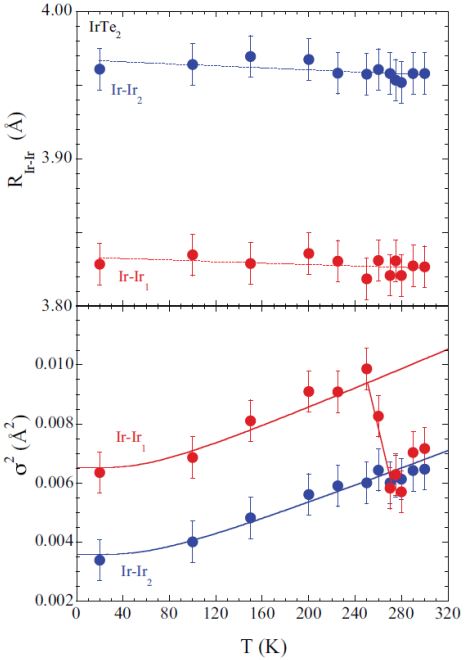
$IrTe_2$: local fluctuating Ir dimers survive at high temperature?!



Ir *L3-edge* EXAFS

B. Joseph *et al.*, PRB (2013)



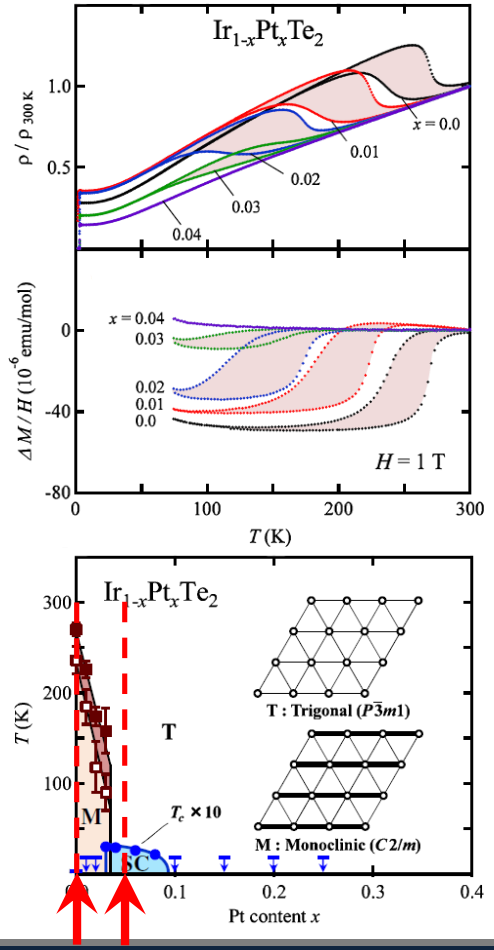


1) Te-dimers and Ir-Te regularize at high-T
2) **Ir-dimers survive locally at high-T**
3) Transition has order-disorder character

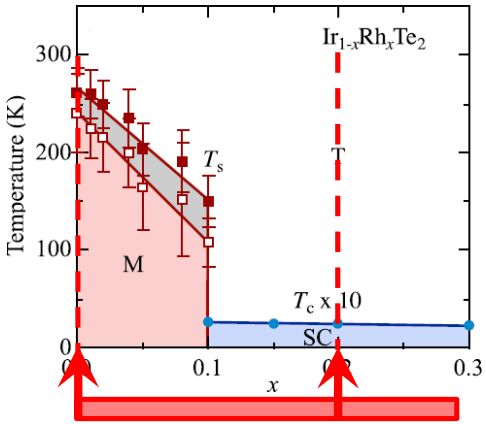
- Interpretation based on C2/m-model
- Early model of LT phase is **wrong**
- **This is not really happening!**

Samples studied: $IrTe_2$, $Ir_{1-x}Rh_xTe_2$ $(0<x<0.3)$, $Ir_{0.95}Pt_{0.05}Te_2$

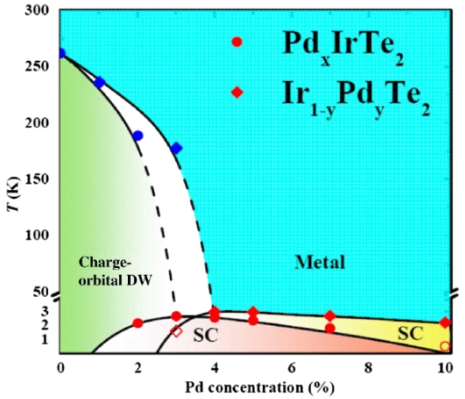
- Reminiscent of unconventional SCs
- Looks like a tunable competition at play
- What is the origin of the LT phase in $IrTe_2$?
- LT phase competes with SC in a QCP-manner?
- Dimer fluctuations involved in the SC mechanism?



S. Pyon *et al.*, JPSJ (2012)

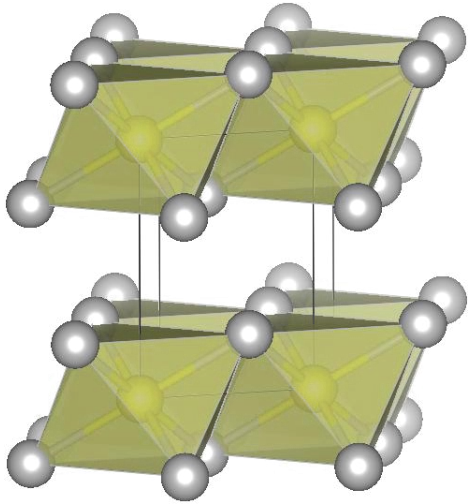


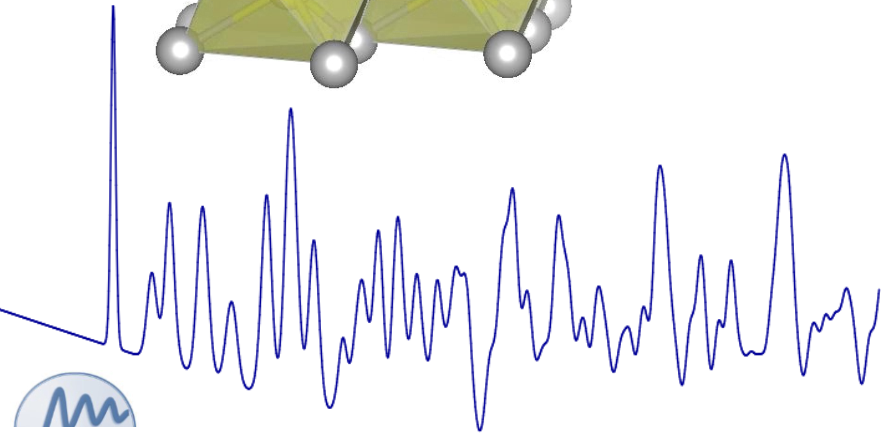
K. Kudo *et al.*, JPSJ (2013)



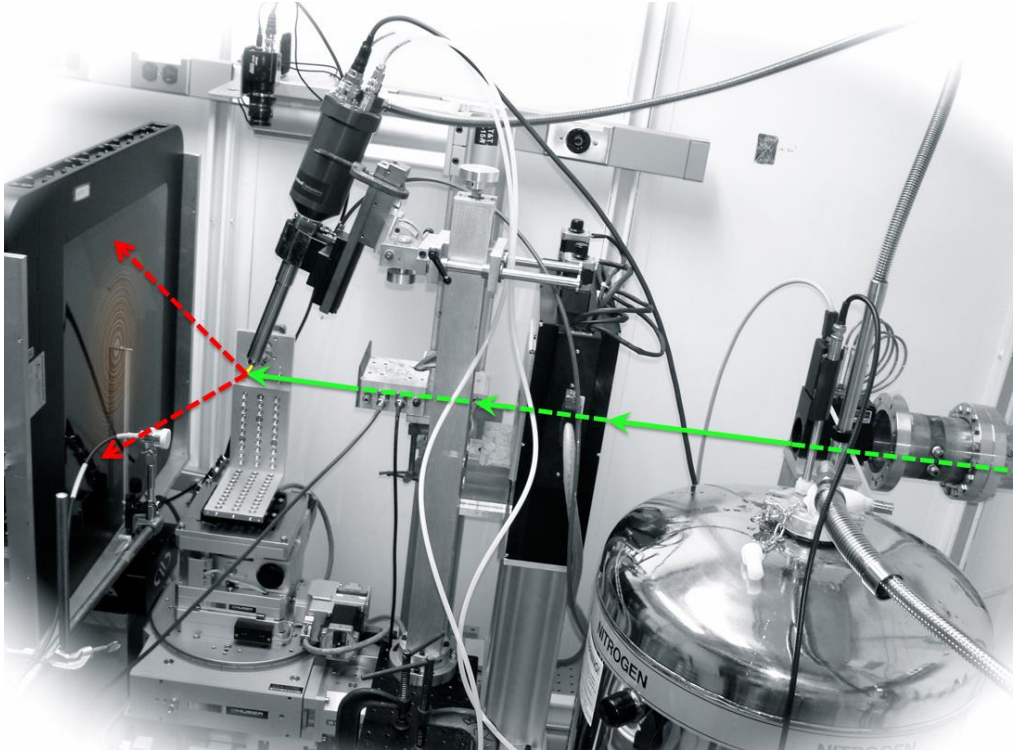
J.J.. Yang *et al.*, PRL (2012)

Experiment: x-ray atomic Pair Distribution Function 10K-300K





interatomic distance, r (Å)



$IrTe_2$, $Ir_{1-x}Rh_xTe_2$ $(0<x<0.3)$, $Ir_{0.95}Pt_{0.05}Te_2$

Detectability of $IrTe_2$ dimers by PDF

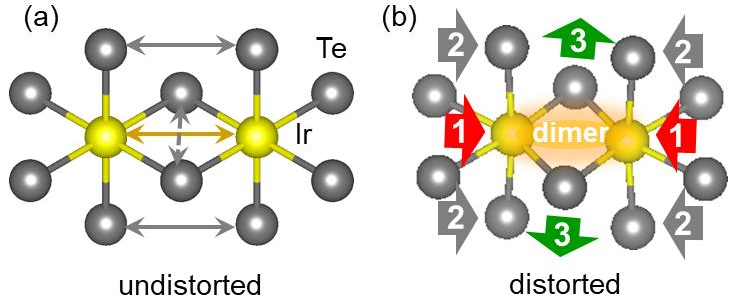
- Dimer associated distortions clearly seen in PDF

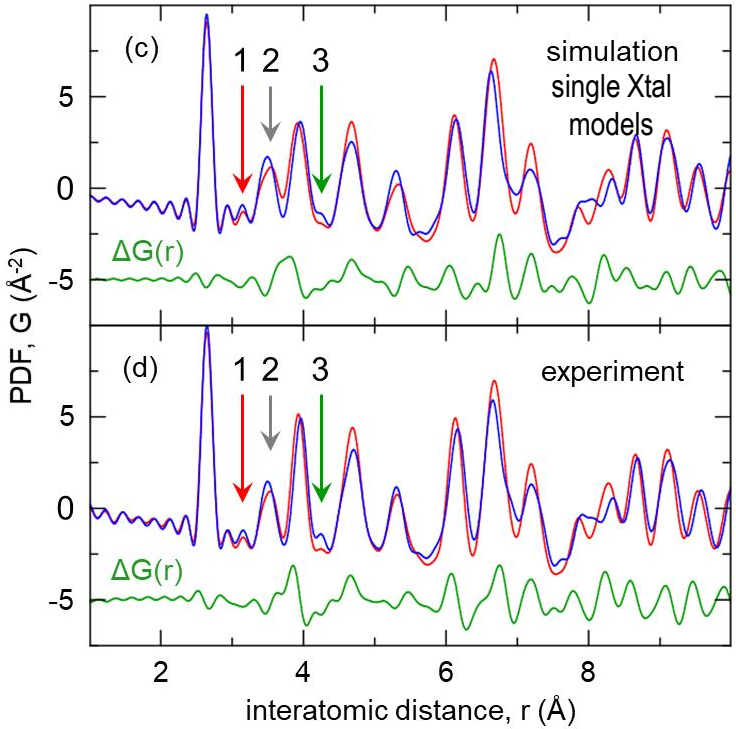
  Δr(Ir-Ir) = -0.8Å *(dimer)*

  Δr(Te-Te) = -0.5Å *(dimer)*

  Δr(Te-Te) = +0.3Å *(lateral)*

- Dimers **disappear** locally in the high temperature metallic phase in disagreement with EXAFS





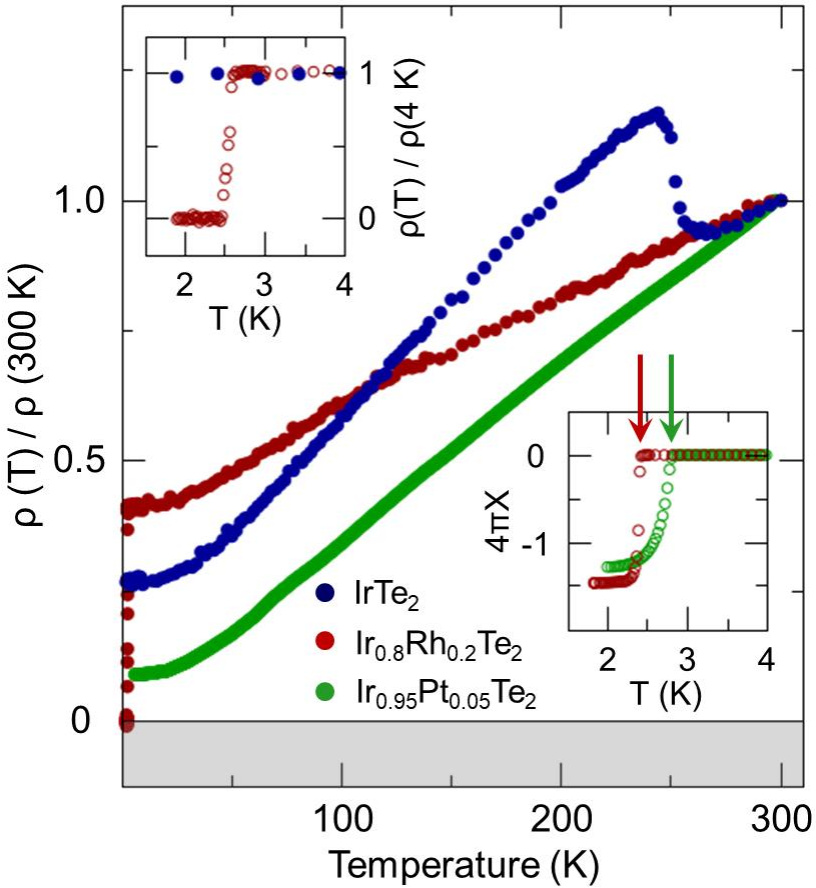
trigonal

triclinic

300K

220K

Properties of the samples studied



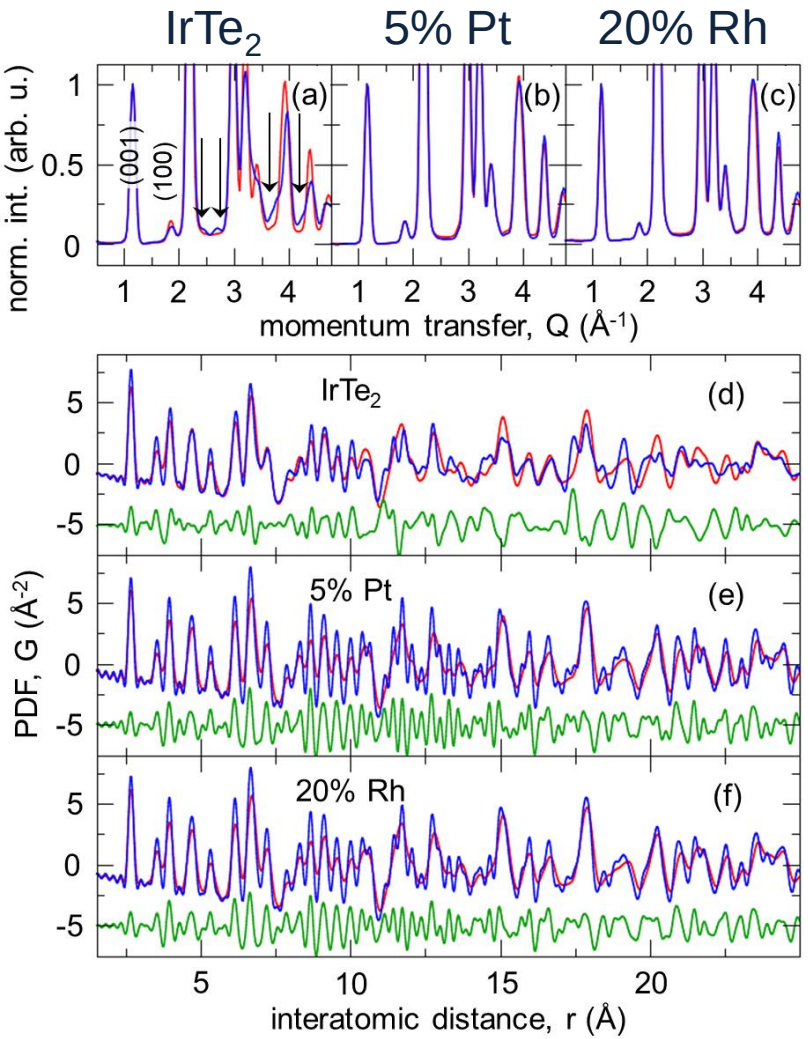
Changes with temperature

Diffraction

- Long range dimer order in $IrTe_2$
- No long range order for SC compositions

PDF

- Short range structure changes in $IrTe_2$
- For SC compositions changes dominantly of thermal origin



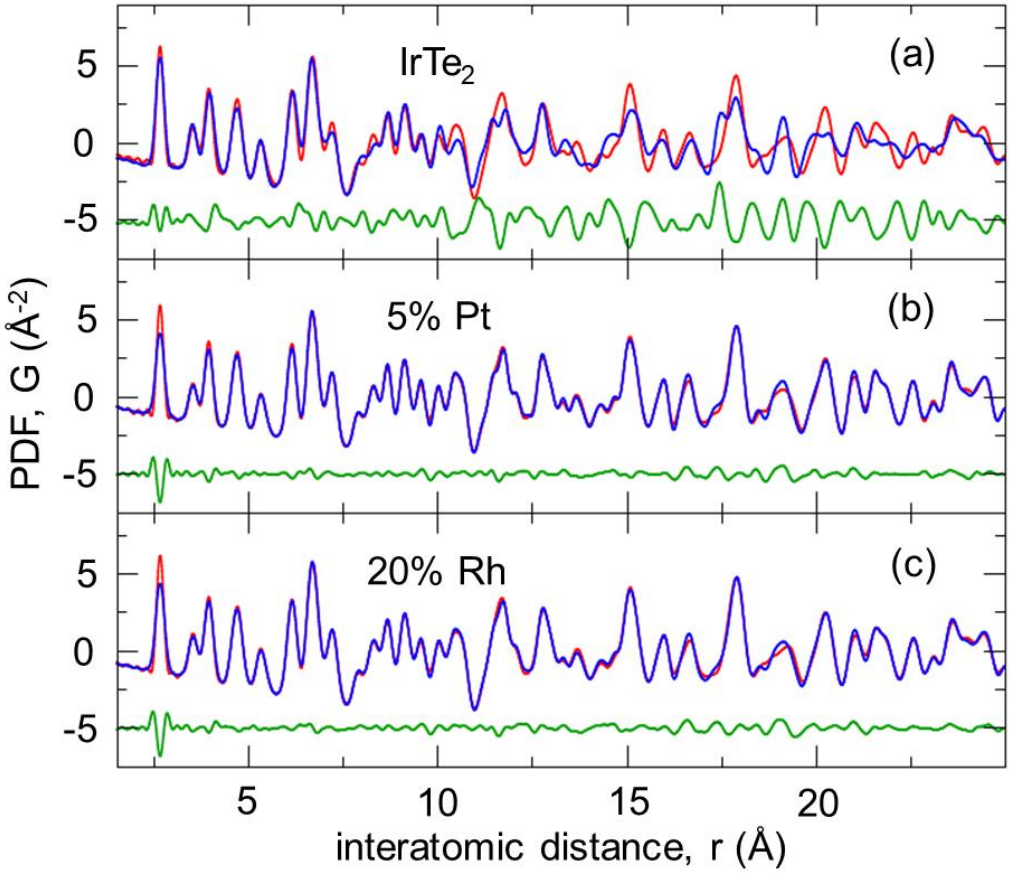
300K

10K

Data morphing (x & y scaling)

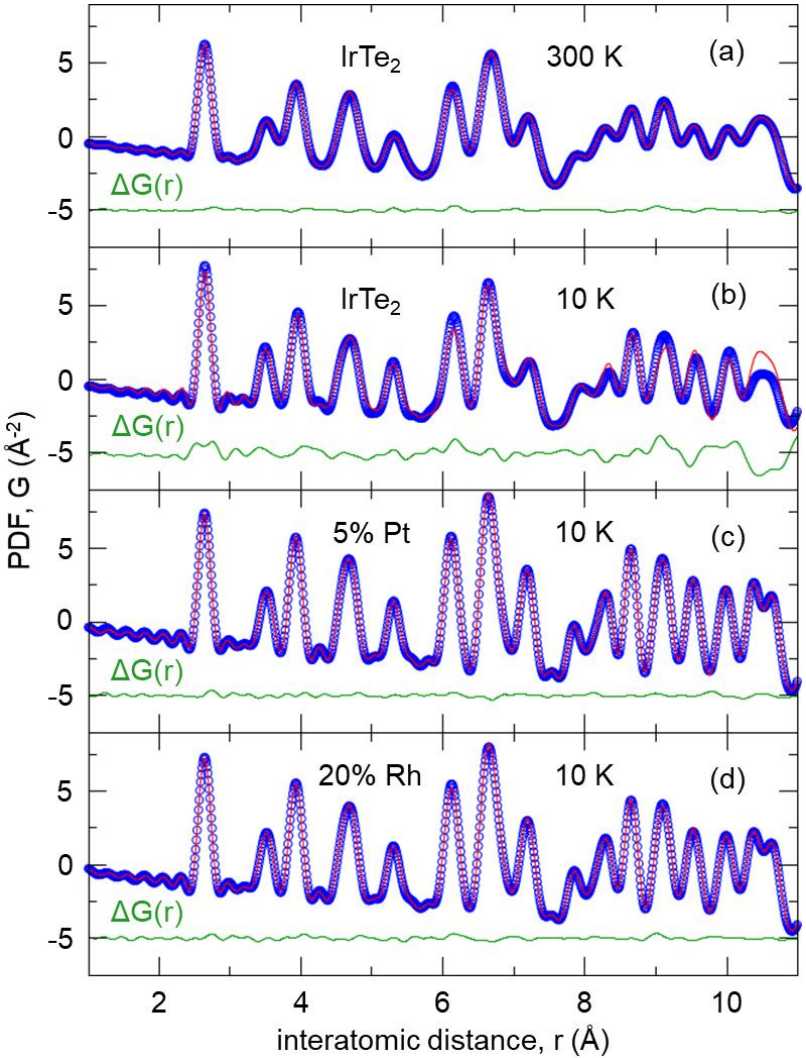
300K 10K

- $IrTe_2$ 300K and 10K data cannot be morphed one onto another
- 5% Pt & 20% Rh data morphable
- For SC compositions changes dominantly thermal in origin



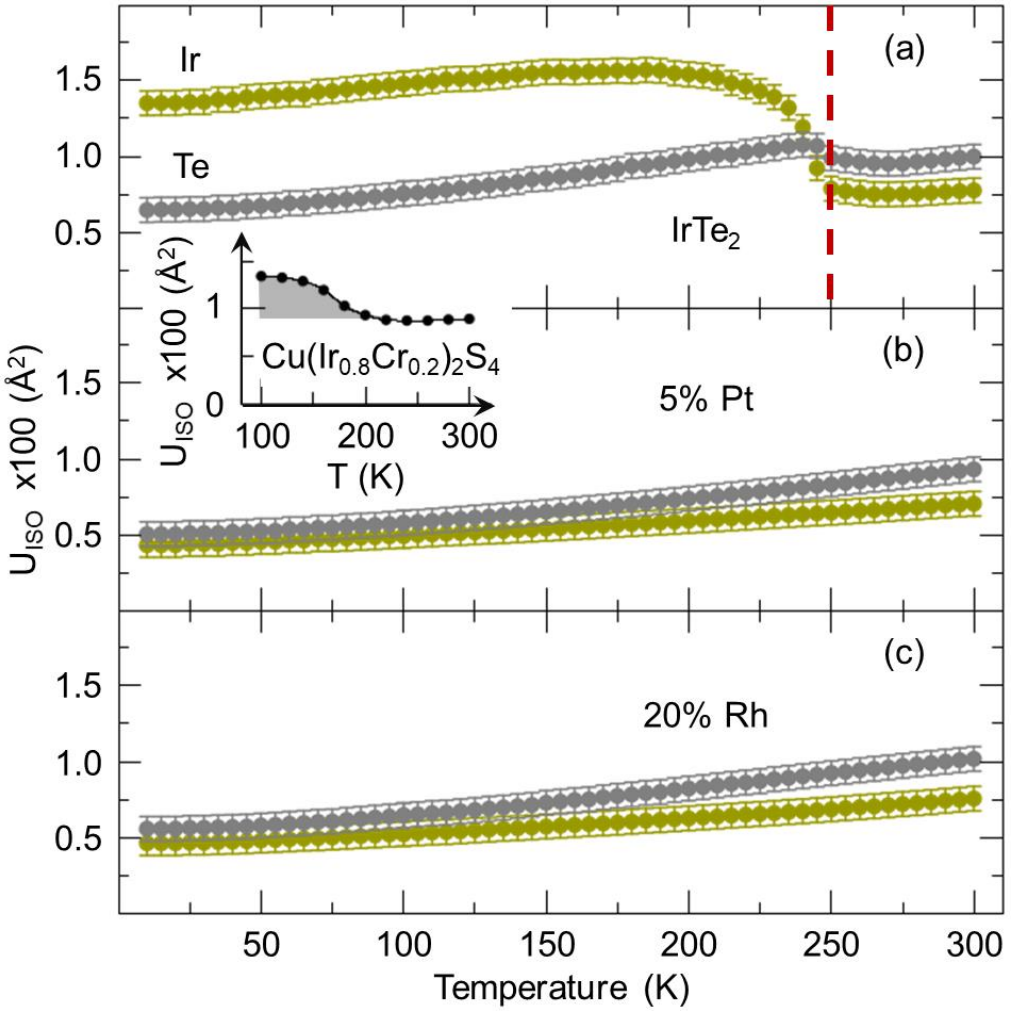
Trigonal high-T model fits

- Fits well $IrTe_2$ data at 300K
- Fails for $IrTe_2$ data at 10K
- Fits well 5% Pt data at 10K
- Fits well 20% Rh data at 10K

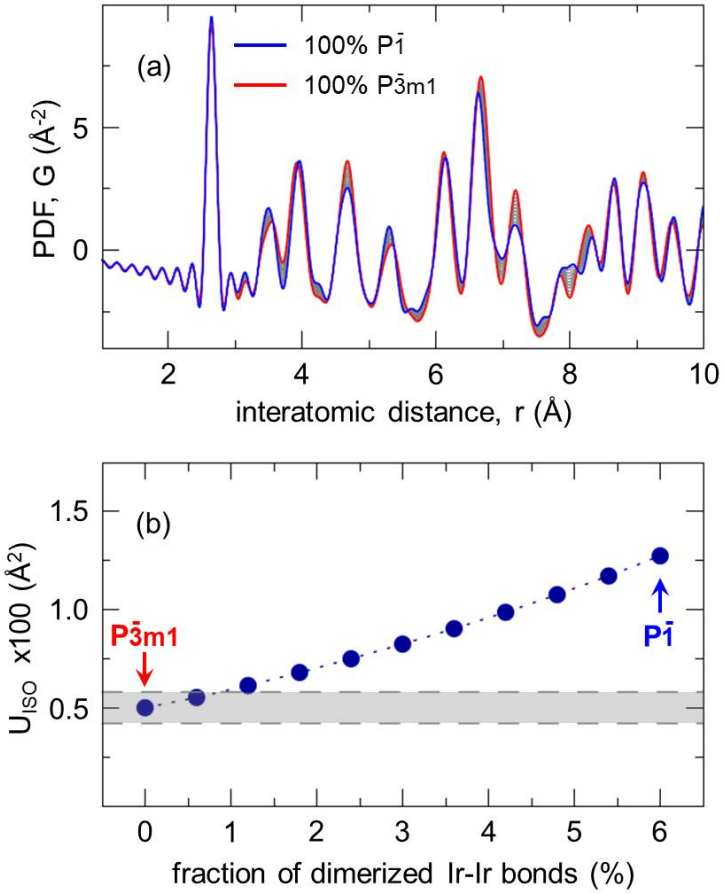


Trigonal model fit results vs temperature

- Upturn in ADPs at the onset T of long range ordered dimers ($IrTe_2$)
- Upturn in Ir-ADPs at the onset T of local fluctuating dimers (Cr-doped $CuIr_2S_4$ spinel)
- No upturn in 5% Pt and 20% Rh substituted IrTe2 down to 10 K
- sensitivity to ~0.5% of dimerized Ir-Ir



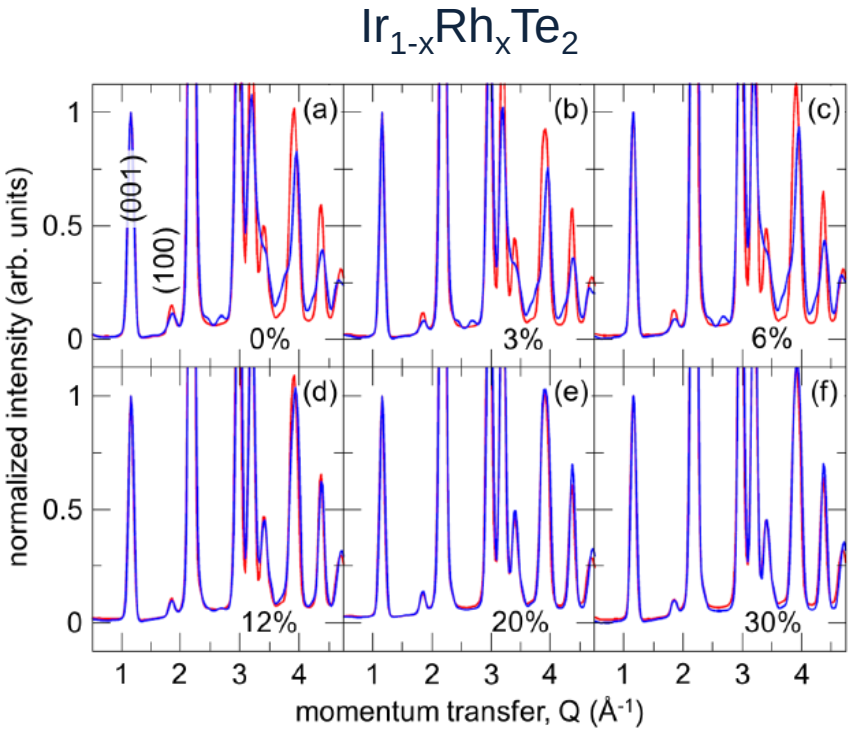
Sensitivity of ADP to the presence of dimers



Changes with Rh-substitution and temperature

Diffraction

- Long range dimer order in $IrTe_2$
- Long range order fading out toward SC Rh-compositions

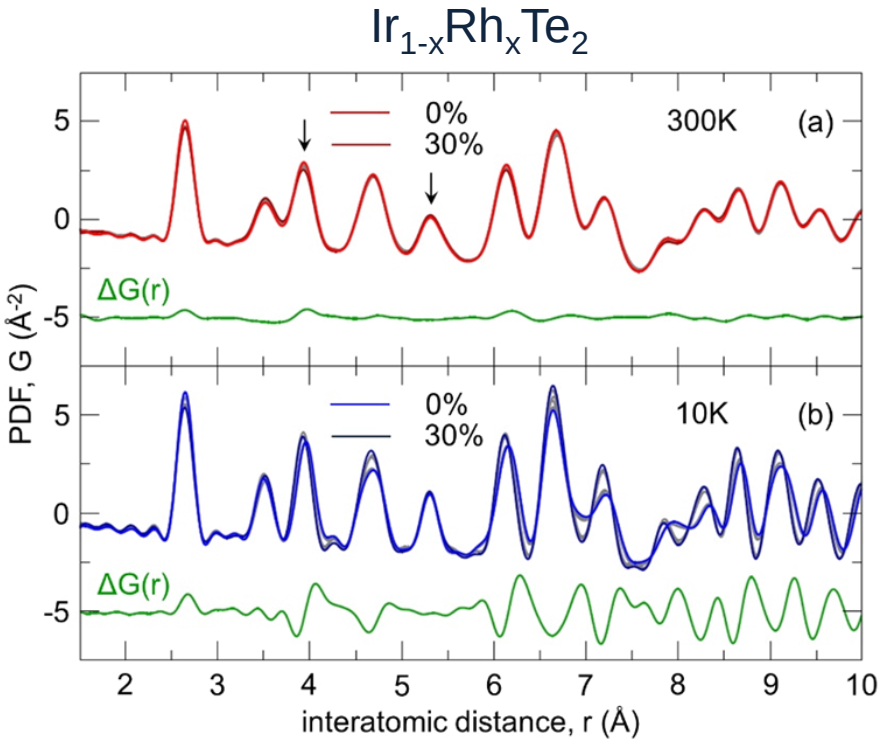


Physical Review B **98**, 134506 (2018)

Changes with Rh-substitution and temperature

PDF

- At 300K all PDFs similar
- At 10K PDFs cluster in two groups

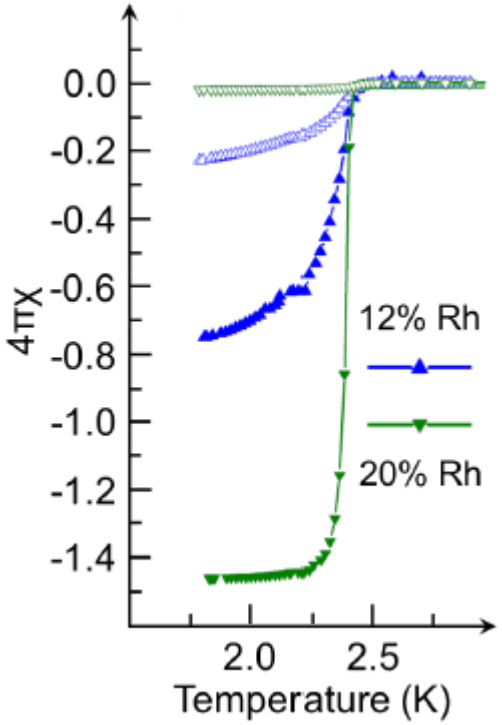


300K

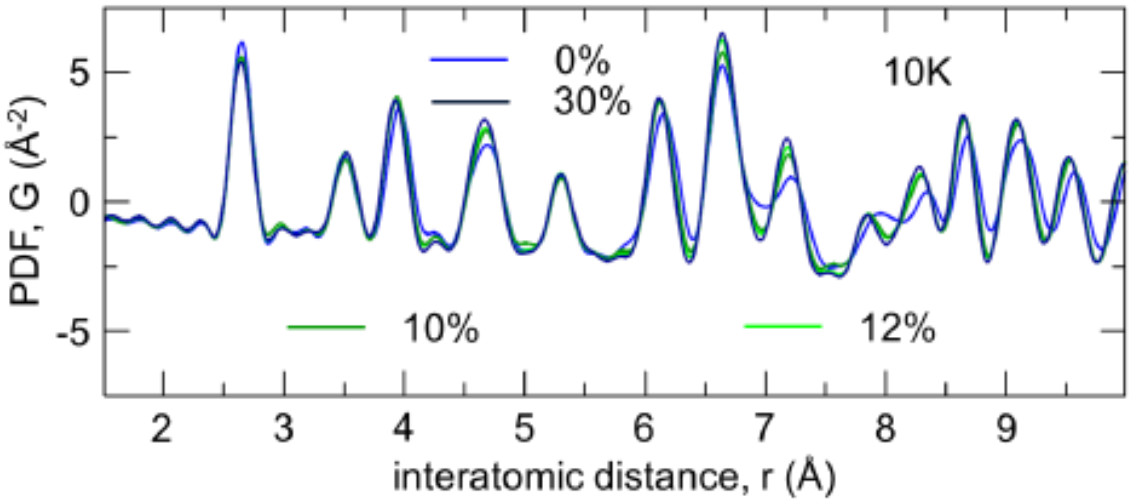
10K

Physical Review B **98**, 134506 (2018)

Low temperature behavior



$Ir_{1-x}Rh_xTe_2$

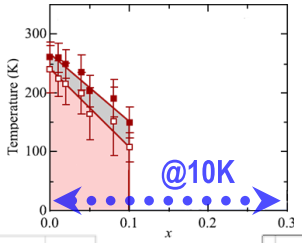


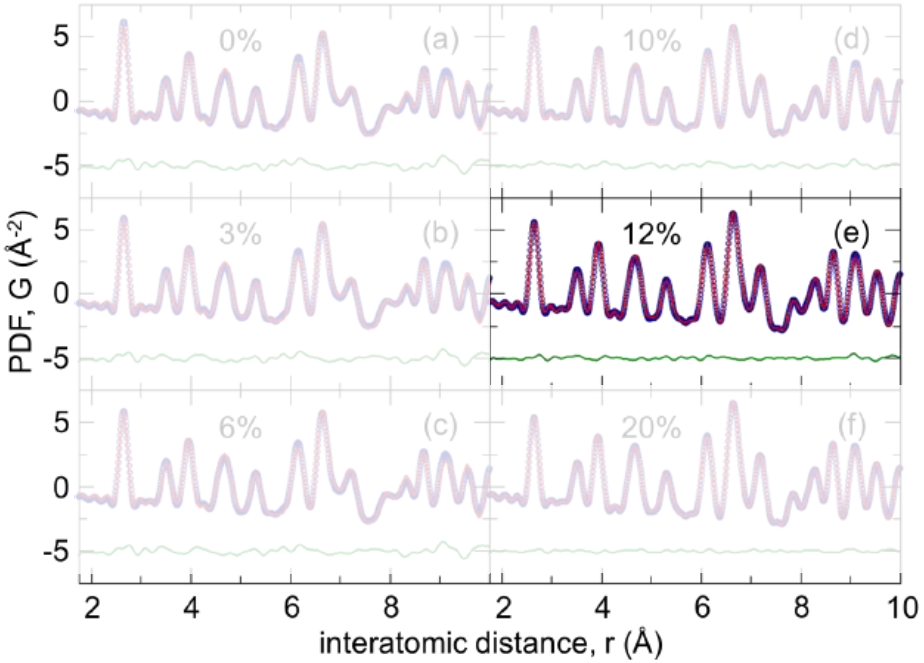
Superconductivity

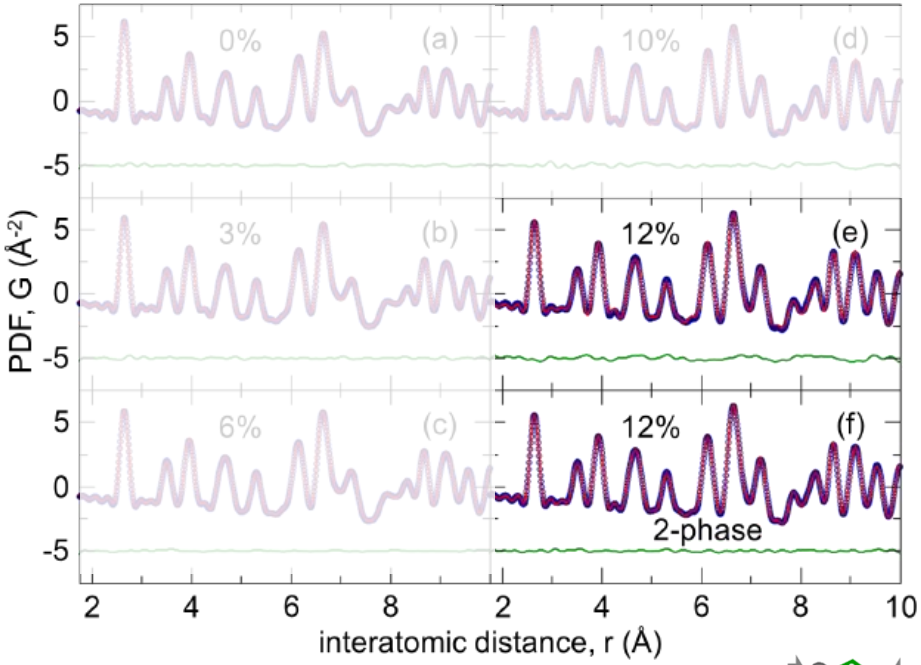
Local structure

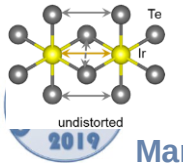
Physical Review B **98**, 134506 (2018)

Structural behavior at 10K



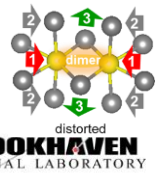






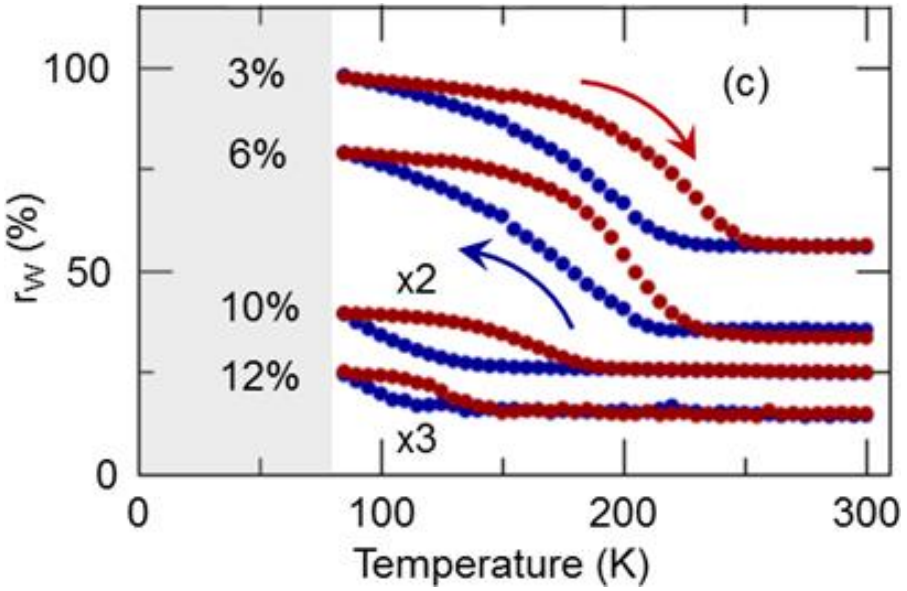
$P\bar{3}m1$ dimer-free model

$P\bar{1}$ dimerized structure model



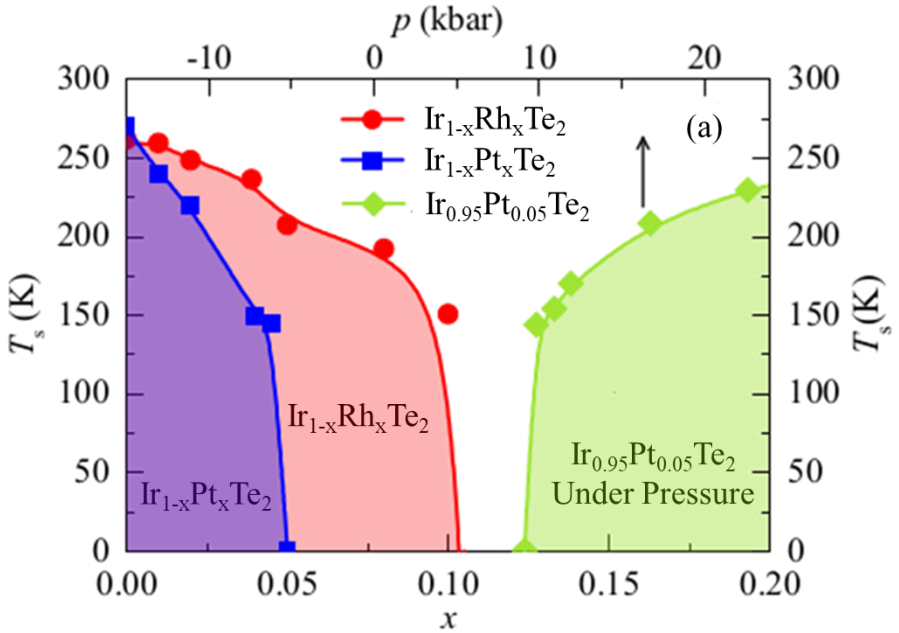
Physical Review B **98**, 134506 (2018)

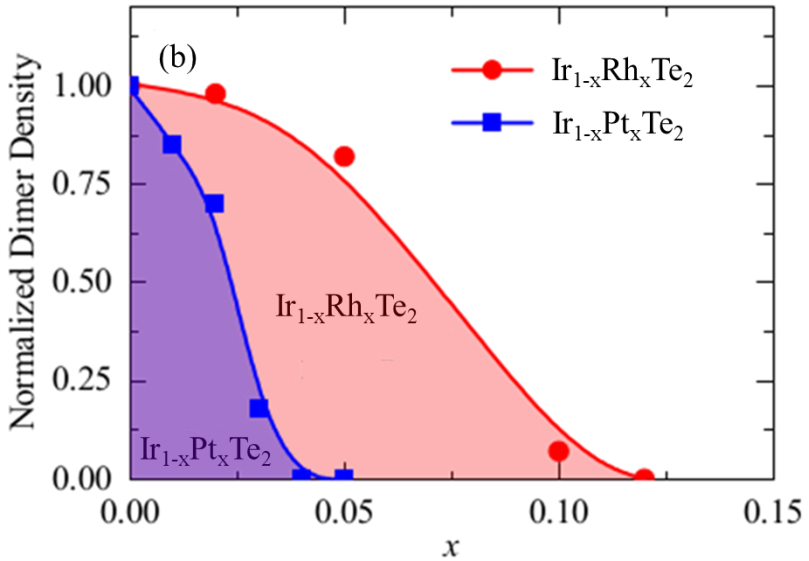
Phase separation in $Ir_{1-x}Rh_xTe_2$ (0<x<0.3)



Physical Review B **98**, 134506 (2018)

Static dimer density & sharpness of the dimer/SC transition





- T_S linear in x
- Sudden drop at dimer/SC boundary
- Similarly, sharp rise with pressure

- From dip in susceptibility
- Gradual depletion with x
- Vanishes for SC compositions

O. Ivashko *et al.*, SciRep (2017)

Physical Review B **97**, 174515 (2018); Physical Review B **98**, 134506 (2018)

Summary

- No evidence for fluctuations of the dimer phase in the SC range of compositions
- No evidence for fluctuating local dimers in the HT phase of $IrTe_2$
- Phase separation close to dimer/SC boundary at 10K
- Dimer/SC transition weakly first order
- **Fluctuating dimers not relevant aspect of the phase diagrams of $IrTe_2$**
- **QCP-scenario for dimer/SC interplay implausible**

Physical Review B **98**, 134506 (2018)
Physical Review B **97**, 174515 (2018)