

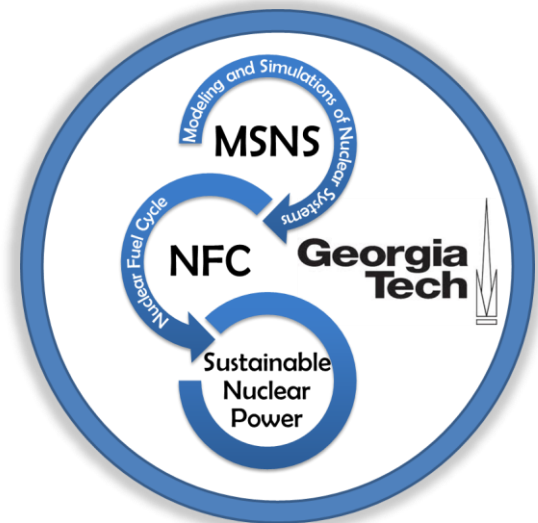
# Numerical Artifacts in Doppler Broadening Near Reference Temperatures

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# Scope of Presentation

## SCOPE

- Study the impact of using different cross section library reference temperatures
  - Conducted ONLY for fuel materials (all other material temperatures and respective references held constant)
  - Quantify impact from using different reference temperatures and characterize resulting behavior

## FINDING

- While conducting this study, some unexpected behaviors were observed (referred to here as “numerical artifacts”)

# Overview



- Introduction
- 2D fuel assembly models
  - One FHR and two PWR models
- Approach
- Results
- Conclusions

# Introduction

- Cross sections affected by changes in temperature
  - Doppler shift due to different velocity distribution from thermal motion<sup>1</sup>

$$\bar{\sigma}(v, T) = \sigma_0 \frac{\Gamma_\gamma}{\Gamma} \frac{m}{\sqrt{\pi} v K T} \int_0^\infty \frac{dv_r v_r \Gamma^2}{\Gamma^2 + (\mu v_r^2 - 2E_0)^2} \left[ \exp\left(-\frac{m(v - v_r)^2}{2kT}\right) - \exp\left(-\frac{m(v + v_r)^2}{2kT}\right) \right]$$

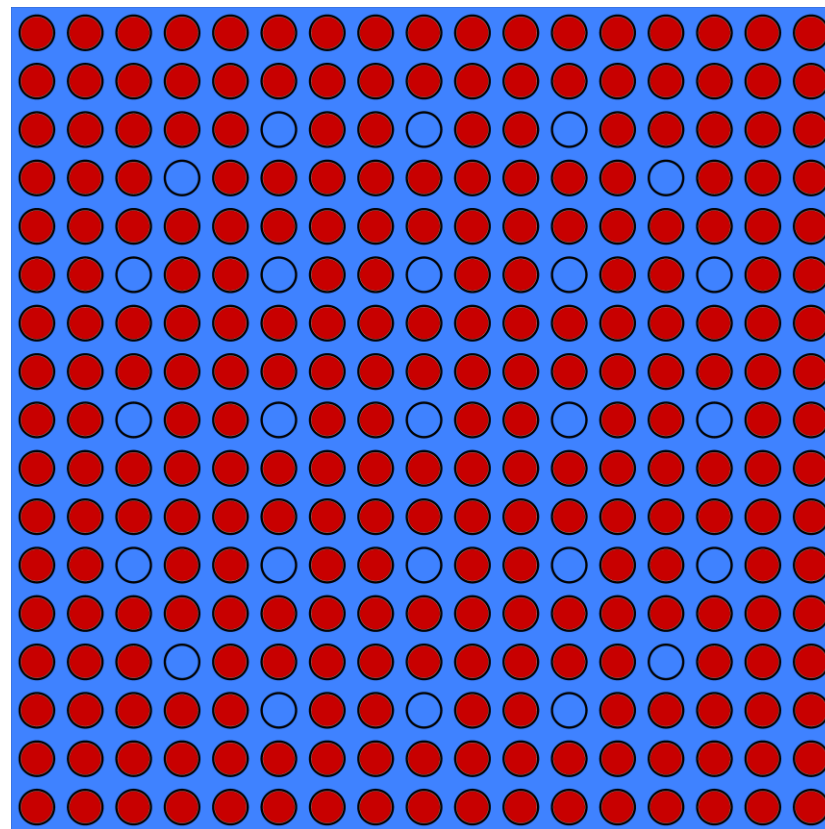
- In codes, cross section libraries contain data in temperature intervals
  - Usually in 300 K increments
  - Material temperatures different from these reference temperatures require the broadening of cross sections in the libraries

<sup>1</sup> J. J. DUDERSTADT, L. J. HAMILTON, *Nuclear Reactor Analysis*, John Wiley & Sons, Inc. (1976) p. 48.

# Model 1 – Standard 17x17 PWR

- Standard Westinghouse 17x17 PWR fuel assembly
- 2D reflected assembly

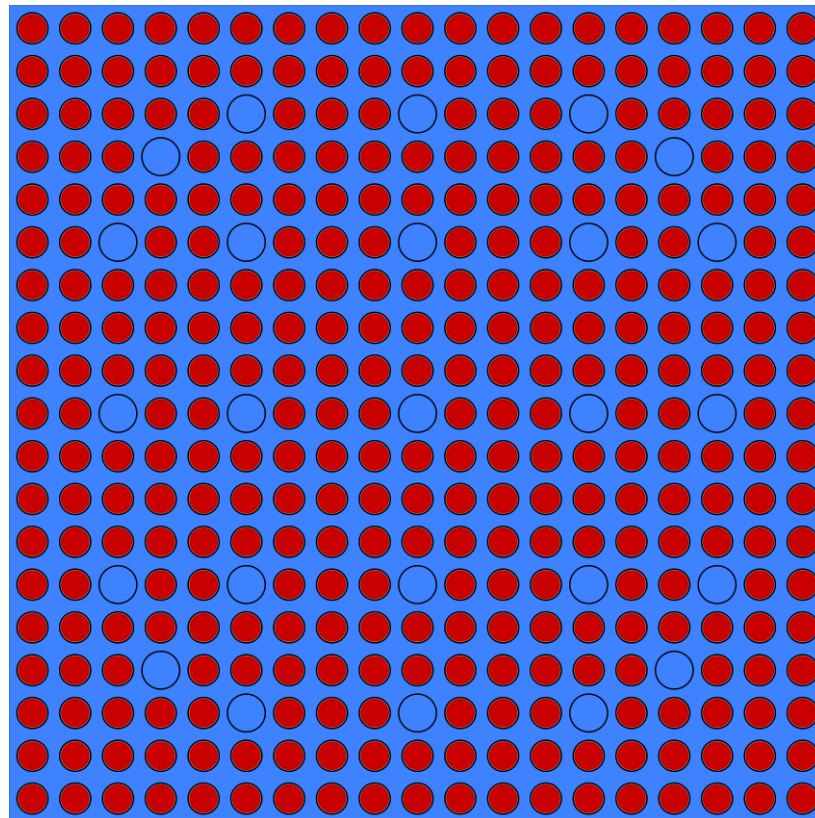
Fuel Radius	0.4095 cm
Gap Radius	0.4178 cm
Clad Radius	0.475 cm
Pin Pitch	1.254 cm
Assembly Pitch	10.7 cm
Enrichment	4.95 w%
Fuel Density	10.52 g/cm <sup>3</sup>
Water Density	0.73 g/cc
Water Temp	580 K



# Model 2 – I<sup>2</sup>S-LWR

- 19x19 U<sub>3</sub>Si<sub>2</sub> fuel with advanced FeCrAl stainless steel cladding<sup>2</sup>
- 2D reflected assembly

Fuel Radius	0.40513 cm
Gap Radius	0.41656 cm
Clad Radius	0.4572 cm
Pin Pitch	1.21006 cm
Assembly Pitch	11.55 cm
Enrichment	4.00 w%
Fuel Density	11.773 g/cm <sup>3</sup>
Water Density	0.7134 g/cc
Water Temp	580 K



<sup>2</sup>B. PETROVIC, "Integral Inherently Safe Light Water Reactor (I<sup>2</sup>S-LWR) Concept: Extending SMR Safety Features to Large Power Output," *Proc. ICAPP 2014*, Charlotte, NC, April 6-9, 2014, **14311**, 78-85, American Nuclear Society (2014).

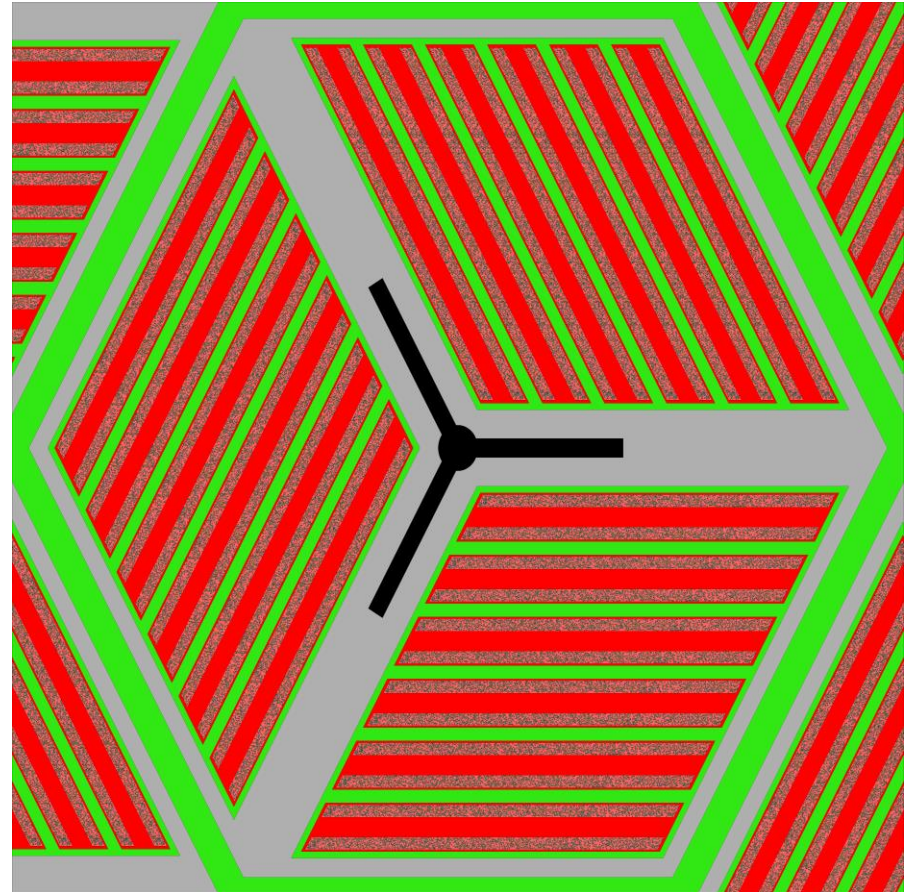


# Model 3 – Prismatic Fluoride-Salt-Cooled High Temperature Reactor (FHR)



- 18 fuel plates per assembly<sup>3</sup>
- TRISO fuel kernels heterogeneously distributed in carbon matrix
- FLiBe liquid salt coolant
- 2D reflected assembly

Fuel Kernel Radius	0.02135 cm
Fuel Enrichment	19.75 w%
Assembly Apothem	22.5 cm
Assembly Pitch	46.75 cm
Fuel Stripe Length	21.32 cm
Fuel Plank Length	21.71 cm
Flow Channel Width	22.52 cm
Coolant Temperature	950 K



<sup>3</sup>B. PETROVIC, G. I. MALDONADO, “Fuel and Core Design Options to Overcome the Heavy Metal Loading Limit and Improve Performance and Safety of Liquid Salt Cooled Reactors,” NEUP Project Final Report (2016).

# Approach

- All analysis done in SERPENT<sup>4</sup> (2.1.27 and 2.1.28)
  - Used the ENDF/B-VII cross section library
- Run cases with the 300K, 600K, 900K, 1200K, and 1500K reference temperatures for fuel materials
  - Look at eigenvalue from 300K-2100K where possible
  - Fuel material temperature must not be less than the reference
- Use two levels of analysis
  - Coarse temperature scale of 100K (for large scale behavior)
  - Fine temperature scale of 1K (for numerical artifact encountered)
- Statistics: most simulations use (unless otherwise stated):  
10<sup>6</sup>/cycle, 100 inactive, 2500 active (~2 pcm uncertainty on k)

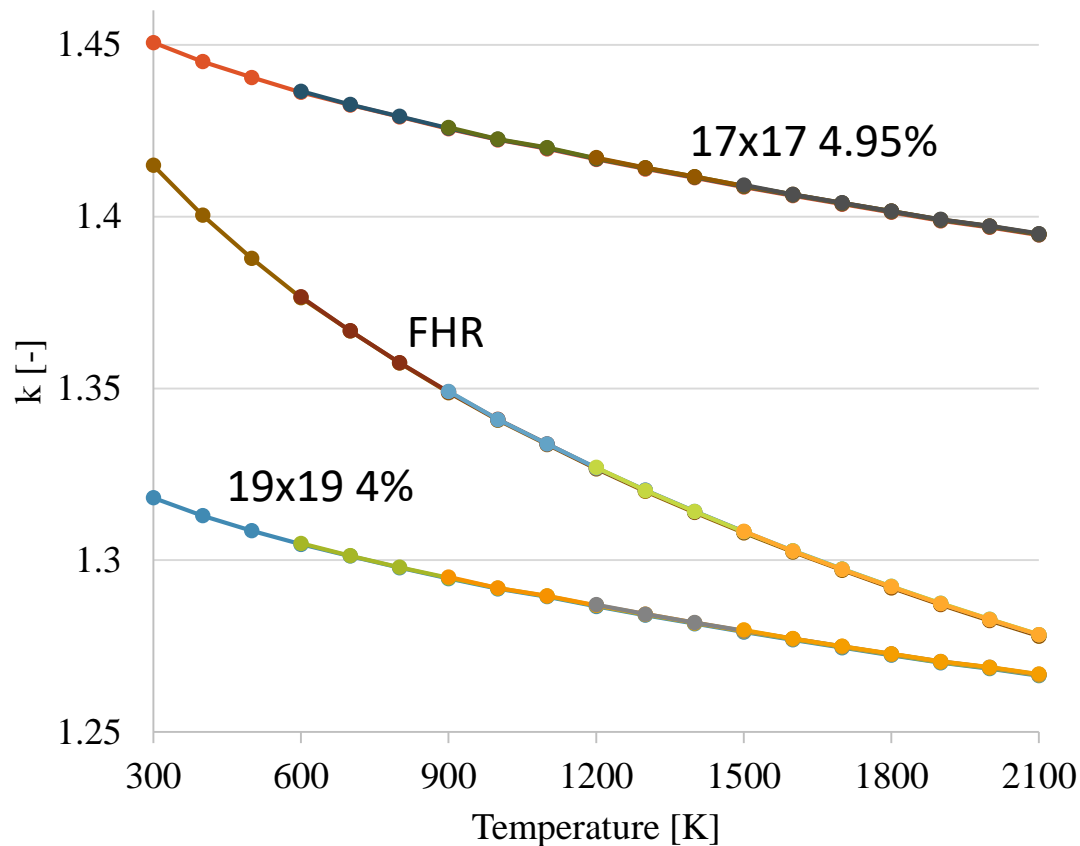
<sup>4</sup>J. LEPPÄNEN, “*Serpent – a Continuous-energy Monte Carlo Reactor Physics Burnup Calculation Code*”, VTT Technical Research Centre of Finland (2013).



# Results-Eigenvalues

- Eigenvalue varying with fuel material temperature using different reference temperatures of each model
- As one would expect, the results appear to be self-consistent on a large scale

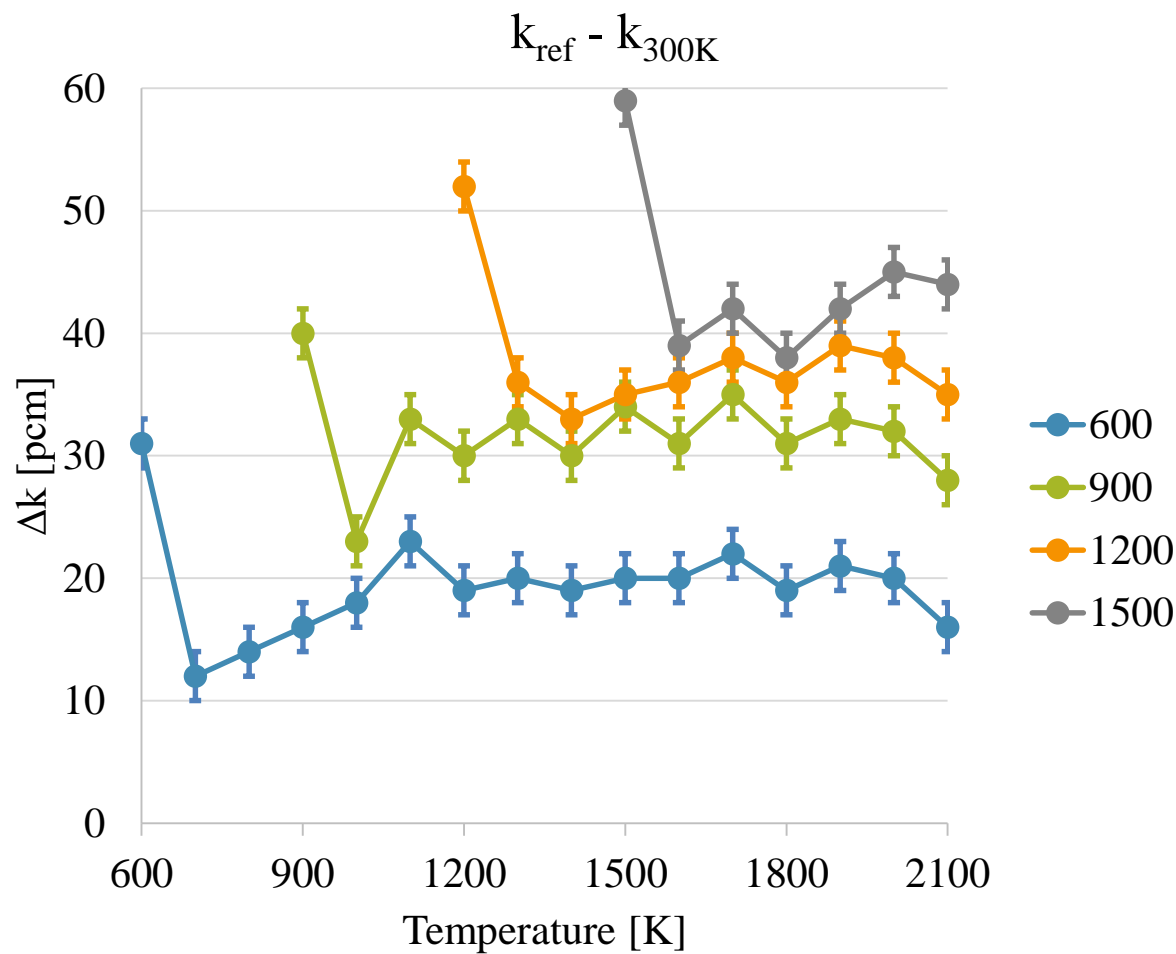
NOTE: some fuel temperatures may not be physical (below coolant temperature, above melting temperature, etc.) but are used to simply capture a large temperature range



# Results – $\text{UO}_2$ Eigenvalue Difference

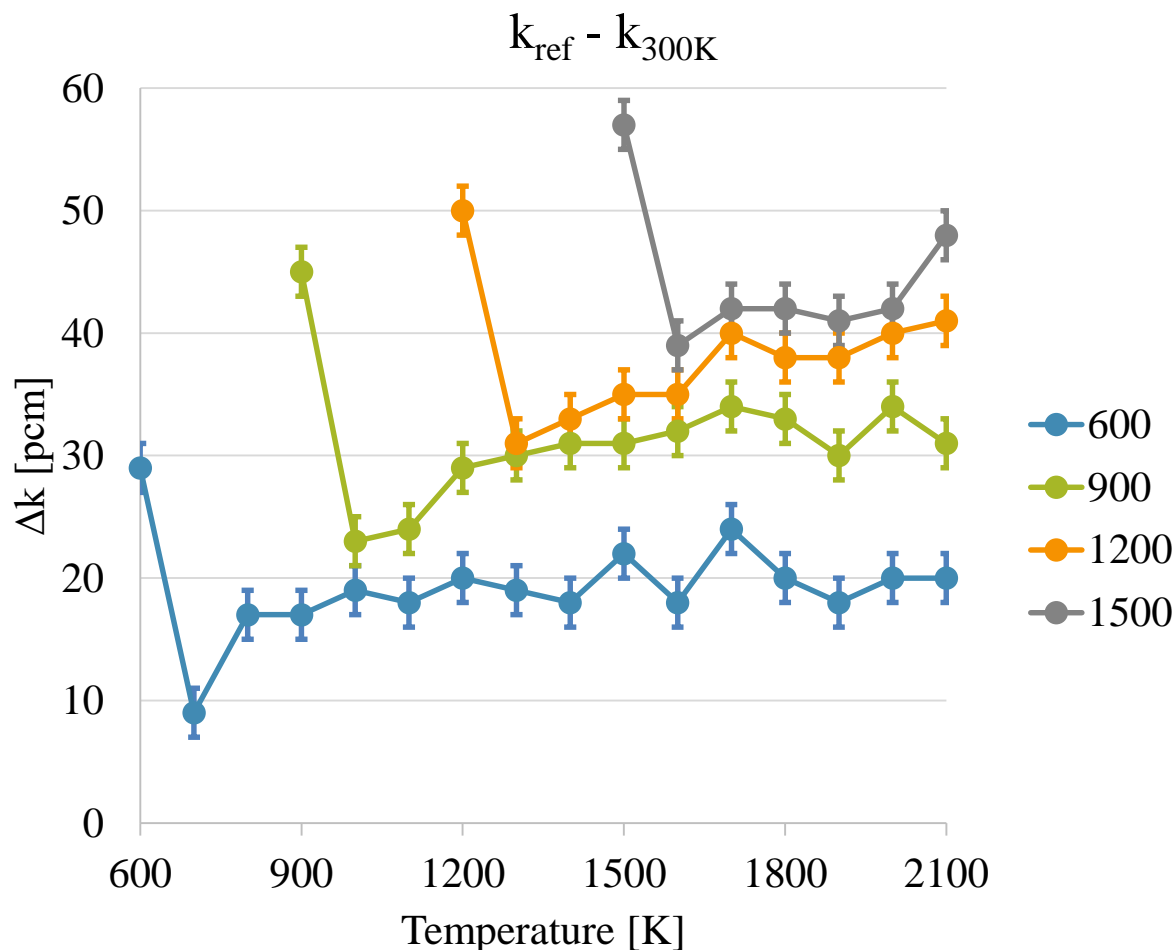
- **Baseline:** results obtained using 300 K cross sections, further Doppler-broadened to other temperatures in the range from 600 K to 2,100 K
- Results also obtained using 600 K, 900 K, 1200 K and 1500 K cross sections, further Doppler-broadened for temperatures above these, up to 2100 K
- The 4 curves show differences against the baseline, for each of the above 4 set of results, in the applicable temperature range (above their reference temperatures)
- Excluding the initial at-reference-temperature point, difference for each curve appears to be weakly increasing with the temperature, i.e., almost flat
- Average differences from the baseline results (excluding at-reference temperatures) increases with temperature:

600 K: 19 pcm  
 900 K: 31 pcm  
 1200 K: 36 pcm  
 1500 K: 42 pcm



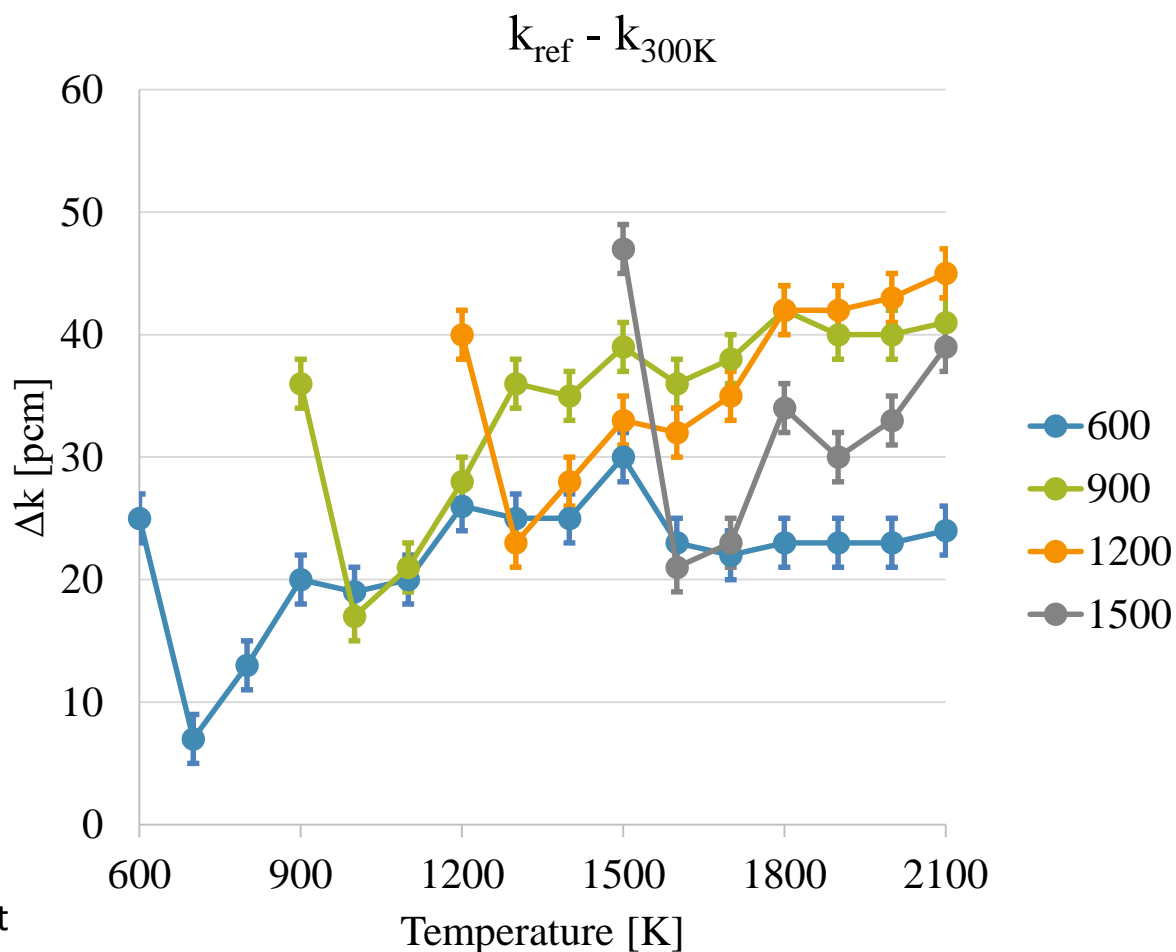
# Results – $U_3Si_2$ Eigenvalue Difference

- Excluding the initial at-reference-temperature point, difference for each curve appears to be weakly increasing with the temperature
- Average differences from the baseline results (excluding at-reference temperatures) increases with temperature:  
 600 K: 19 pcm  
 900 K: 31 pcm  
 1200 K: 37 pcm  
 1500 K: 42 pcm
- Very similar results to Model 1



# Results – FHR Eigenvalue Difference

- Excluding the initial at-reference-temperature point, each curve appears to be increasing with temperature more strongly than for PWR, having a non-trivial slope
- Average differences from the baseline results (excluding at-reference temperatures):
  - 600 K: 22 pcm
  - 900 K: 34 pcm
  - 1200 K: 36 pcm
  - 1500 K: 30 pcm
- The average difference is not monotonically increasing any more.
  - Average difference for 1500 K is smaller than the average difference for 900 K and 1200 K.
  - Not understood why at this point

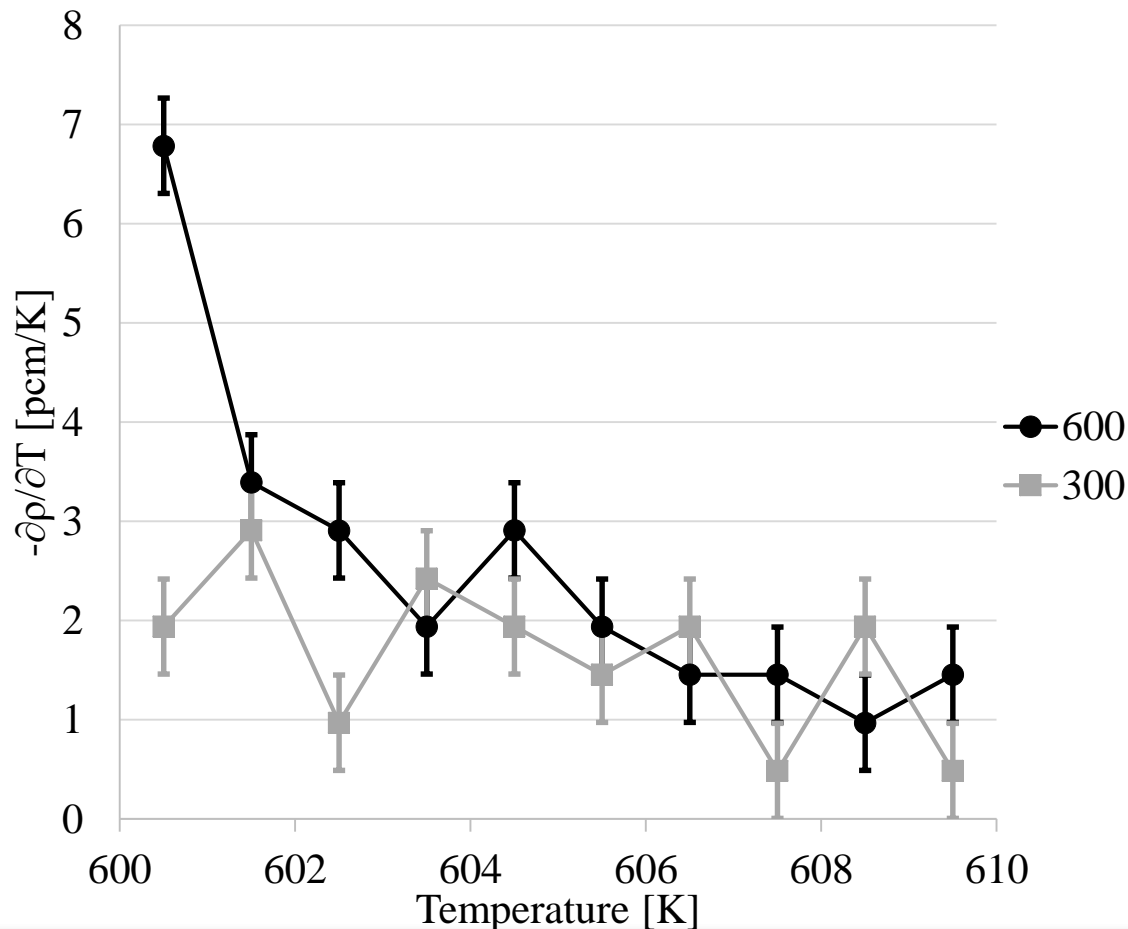


# Finer Temperature Scale

- A numerical artifact appears when the fuel material temperature is the same as its cross section library reference temperature
- To investigate this further, a finer temperature grid was used
  - 1 K instead of 100 K

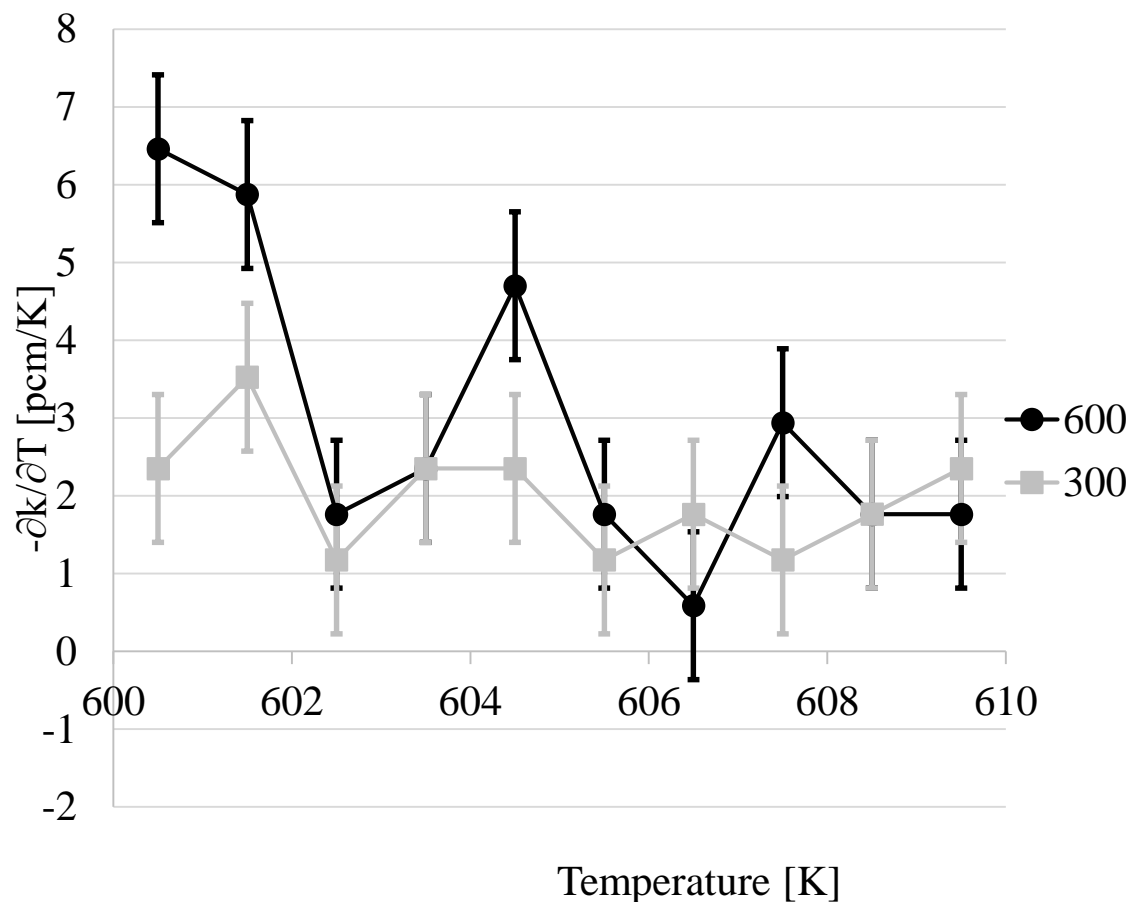
# Results – $\text{UO}_2$ Fuel Temp. Reactivity Coeff.

- Baseline results (300 K library, Doppler-broadened) give a value of the temperature reactivity coefficient about -2 pcm/K over the whole temperature range 600K-2100K
- 600 K reference has large difference close to 600 K, but drops to near the expected value of -2 pcm/K quickly (around 603 K)



# Results – $U_3Si_2$ Fuel Temp. Reactivity Coeff.

- Similar observations as for the  $UO_2$  case
- Some oscillations above 603K, likely due to relatively large statistical uncertainty\* for such a small temperature difference

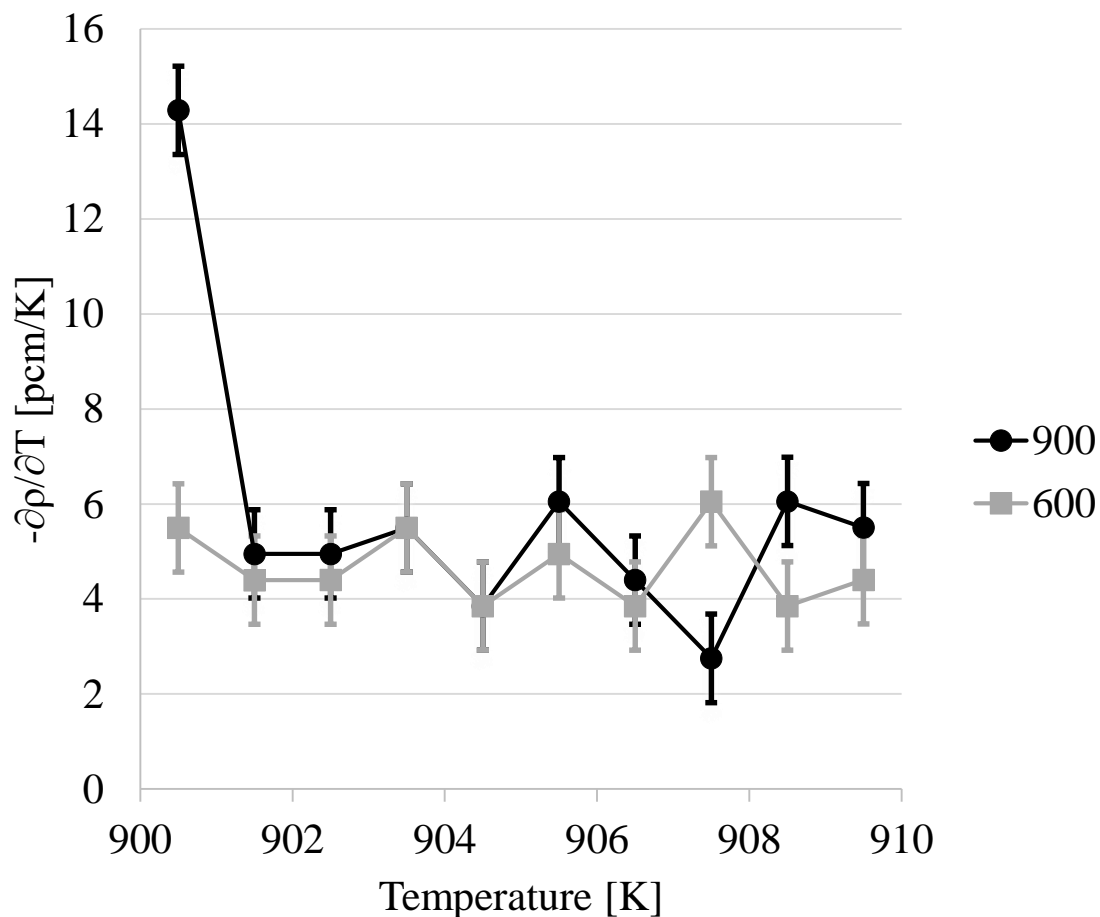


\*Run using only 1E6 part/gen, 500 inactive, 2500 active gens

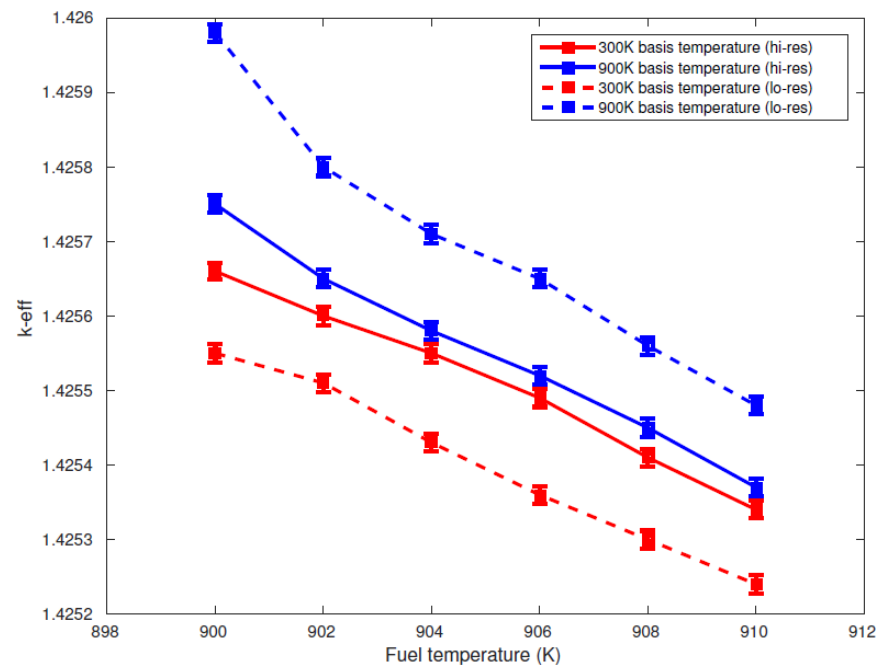


# Results – FHR Fuel Temp. Reactivity Coeff.

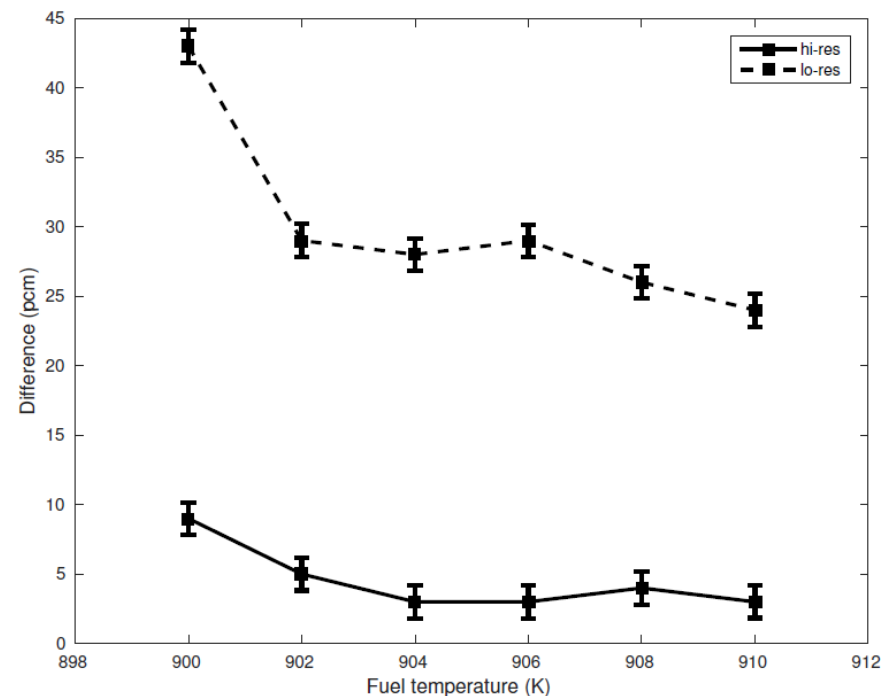
- Baseline results (600 K library, Doppler-broadened) give a value of the temperature reactivity coefficient about -5 pcm/K over the whole temperature range 900 K - 2100 K (as expected based on the coarse temperature grid results)
- 900 K reference has large difference close to 900 K, but drops to expected value quickly (by 902 K)



# Possible Explanation: Cross Section Library Energy Resolution<sup>5</sup>



- Results obtained with higher energy resolution [solid lines using a lower thinning tolerance] more similar than lower energy resolution [dashed lines] (which is distributed)



- Improvement seen with using higher resolution
- However, higher resolution still sees the same artifact, to approximately the same relative degree

<sup>5</sup>J. Leppänen. Personal correspondence. October 27, 2017.

# Summary of Findings

- Away from the numerical artifacts (i.e., except when the fuel temperature matches the cross section library reference temperature), all three models have eigenvalue differences less than 50 pcm
  - Even comparisons between 300 K and 1500 K
  - As included with each model's results, these differences are predictable (depending on the type of system – analysis would need to be repeated for different designs)
- Non-physical behavior observed
  - Numerical artifacts, on the order of 20 pcm, are likely a consequence of the cross section energy resolution
  - Exact reason still uncertain – further investigation needed

# Conclusions

- Results are ultimately a curiosity; negligible for most studies
  - Can be too small to be relevant or materials not near their reference temperatures
- However, in cases where small changes are important, need to be aware if the sought result is near a reference temperature
  - Frequently encountered in benchmark definitions – can be exactly at the Doppler reference temperature
  - Results may be impacted by numerical artifact up to about 20 pcm for PWR systems

However, other systems may see a larger impact

Potential future work:

- Additional studies and examination of the formulation to clarify the cause and mitigate the artifacts

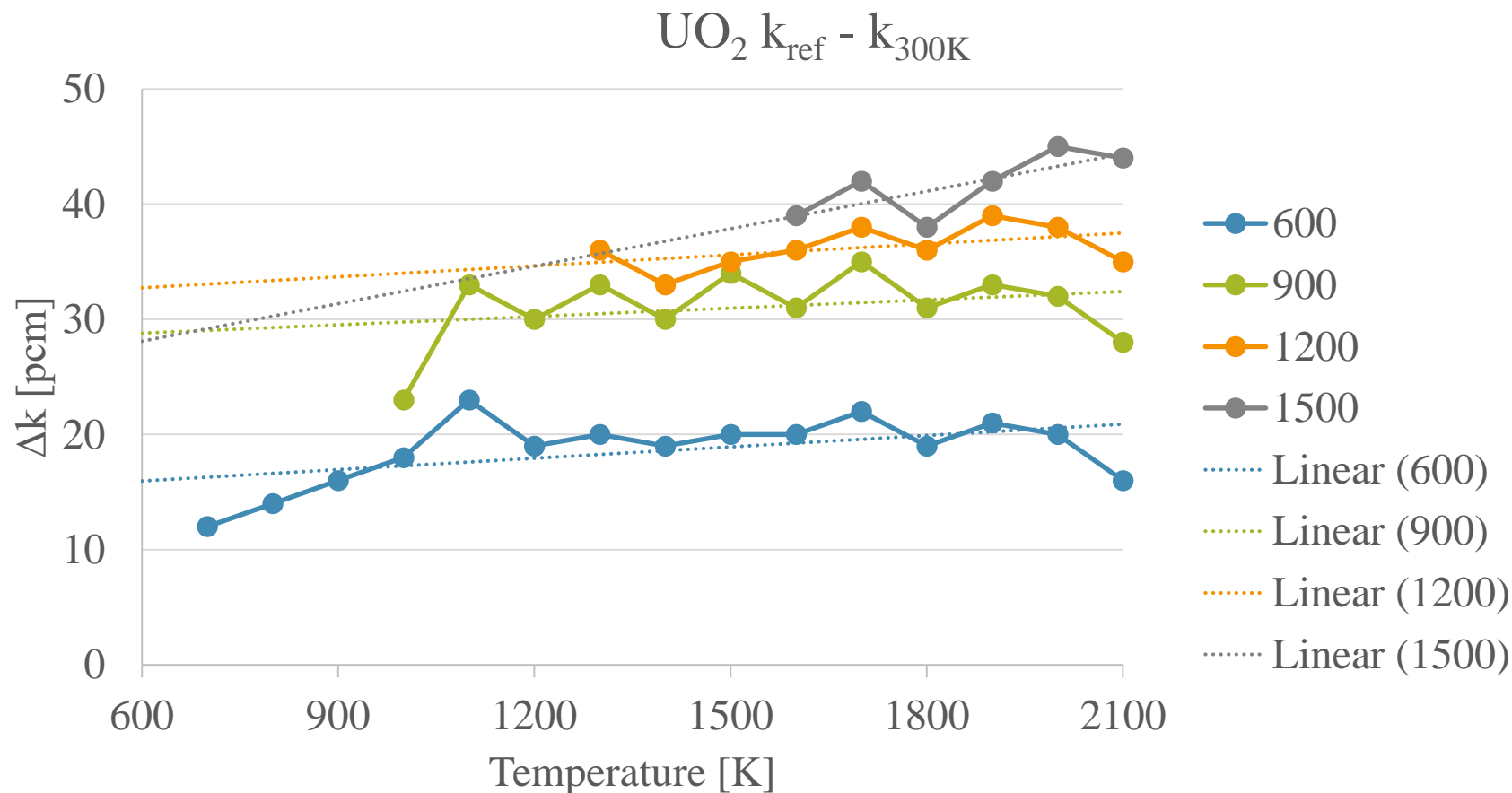
# End of Presentation



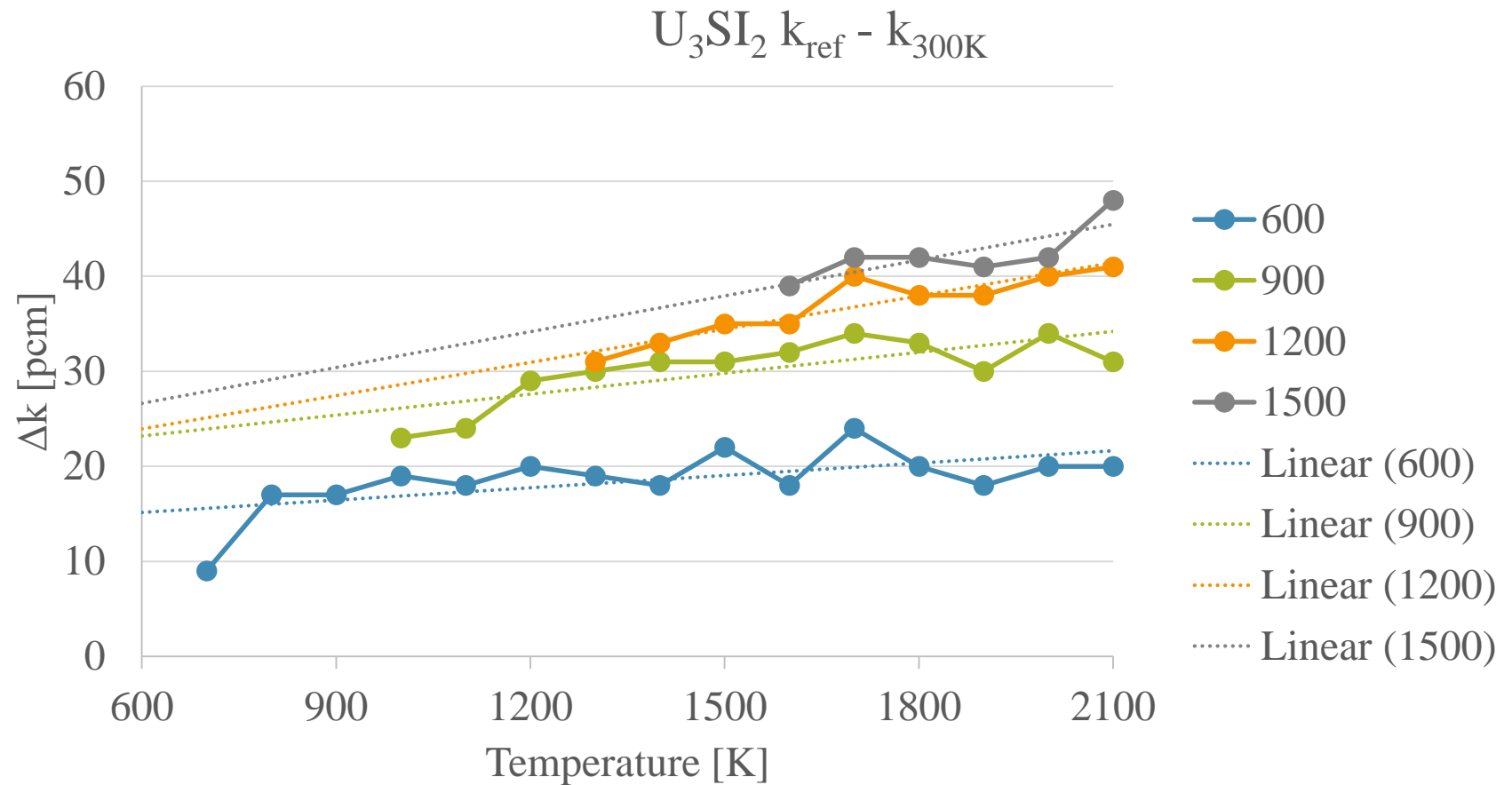
Kyle Ramey (kmramey@gatech.edu)

Thank you for your attention.  
Questions?

# Supplementary

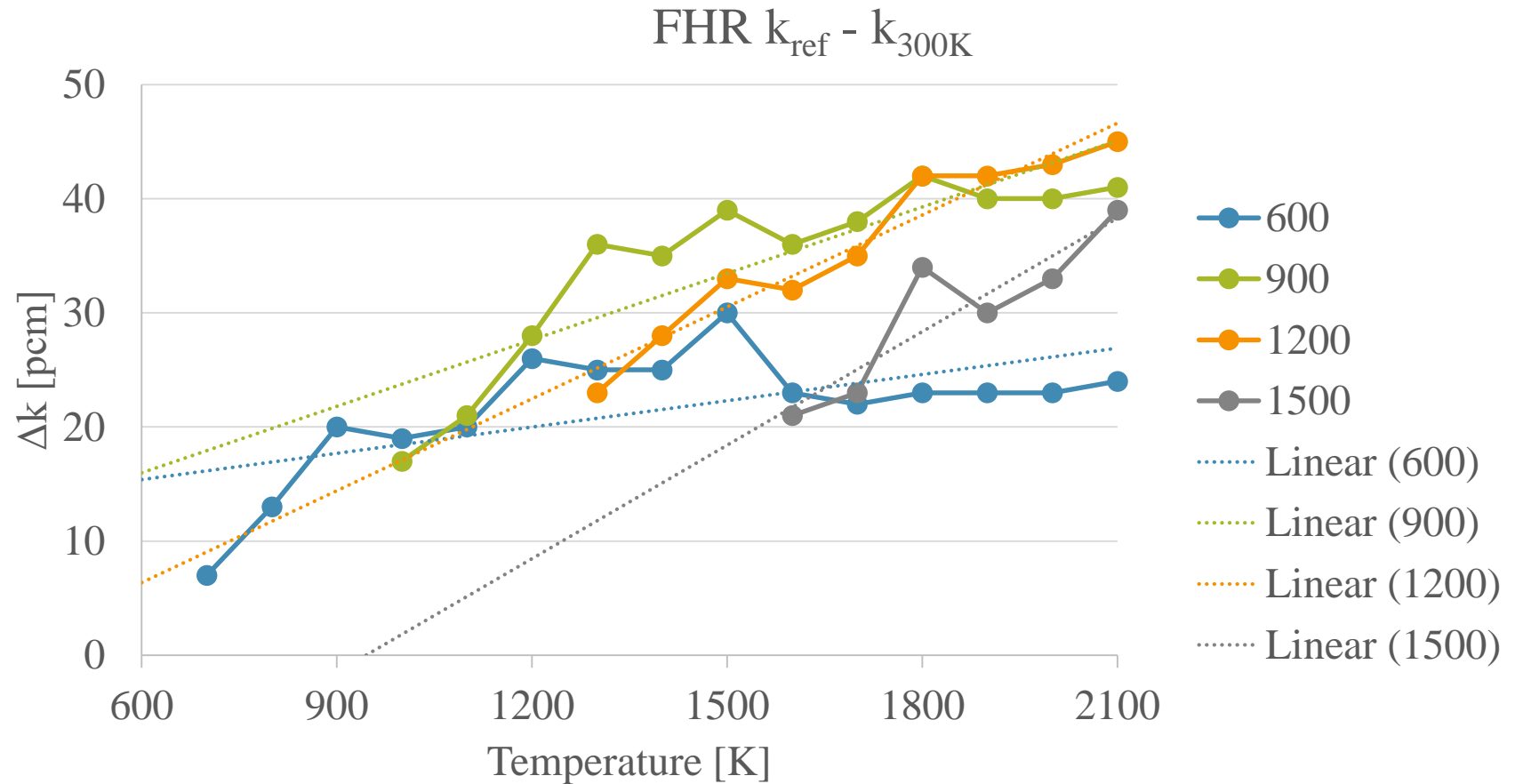


# Supplementary

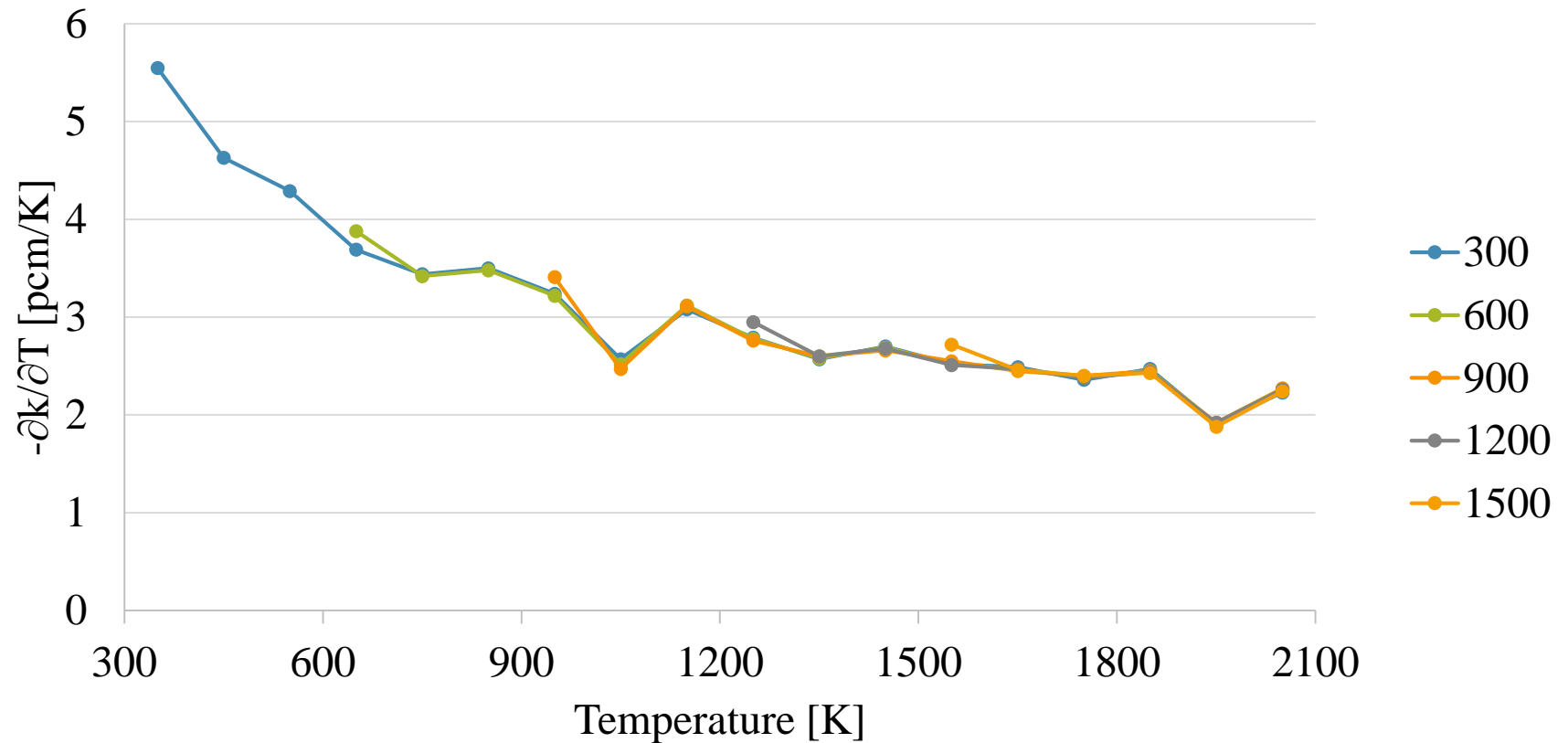




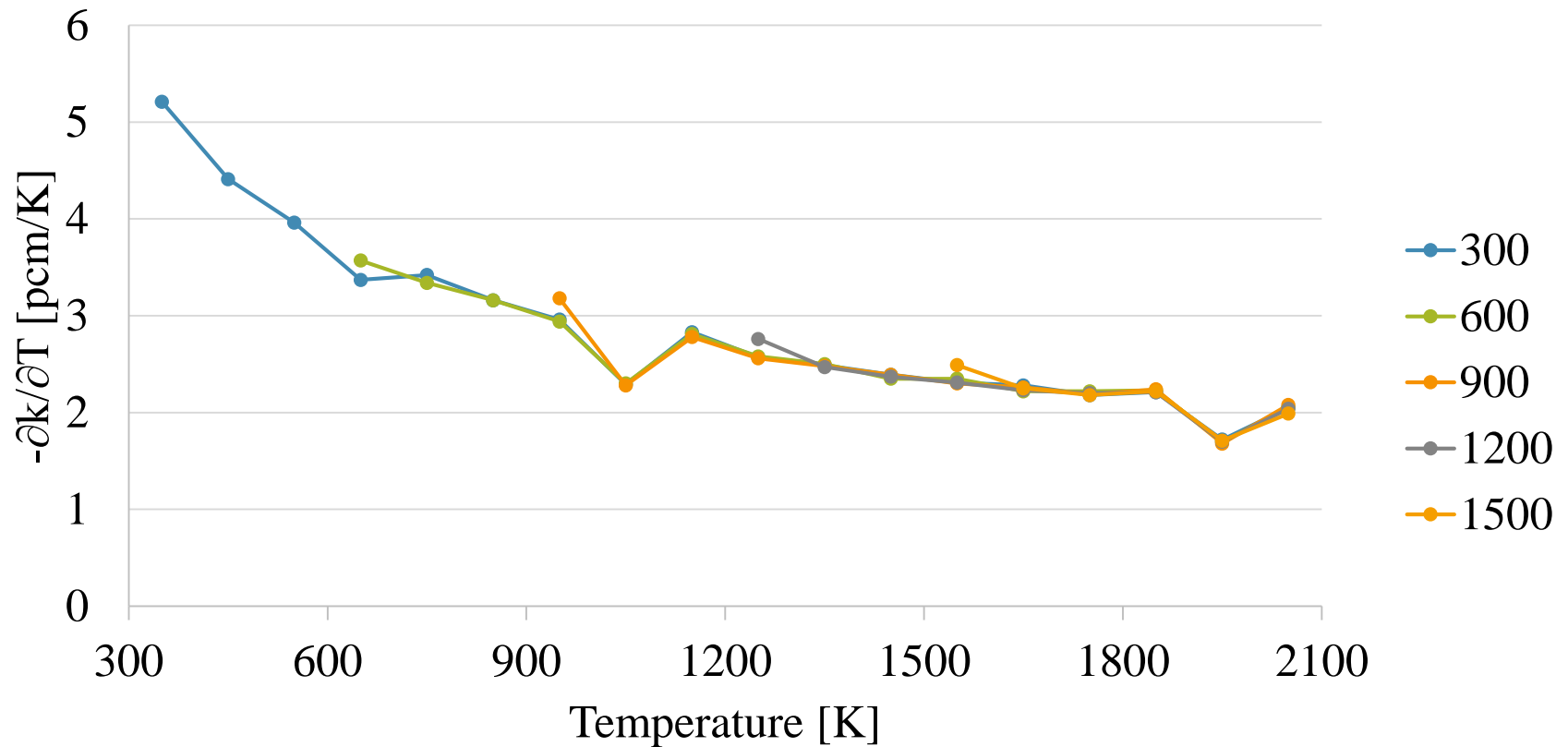
# Supplementary



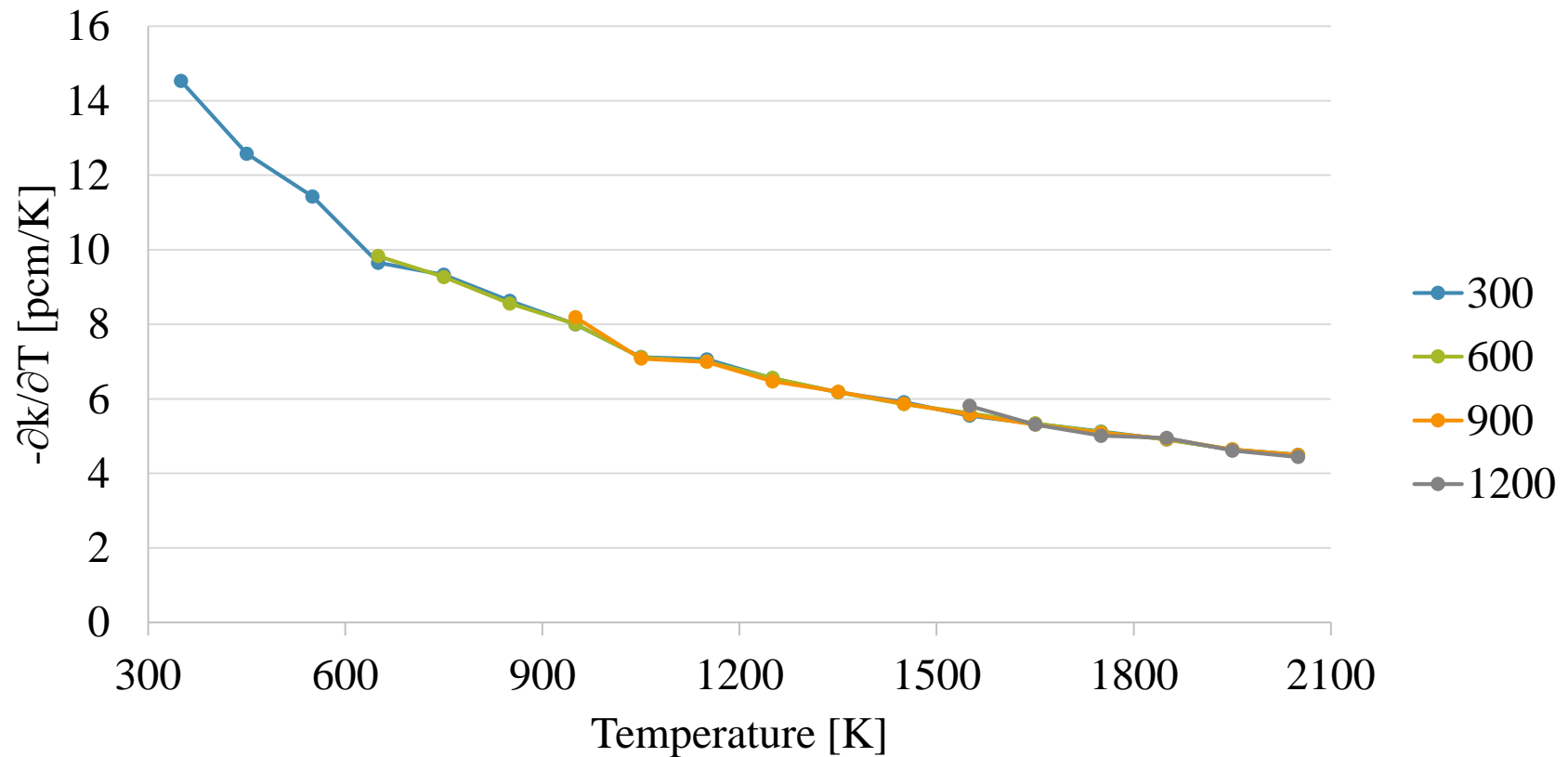
## UO<sub>2</sub> Doppler Coefficient



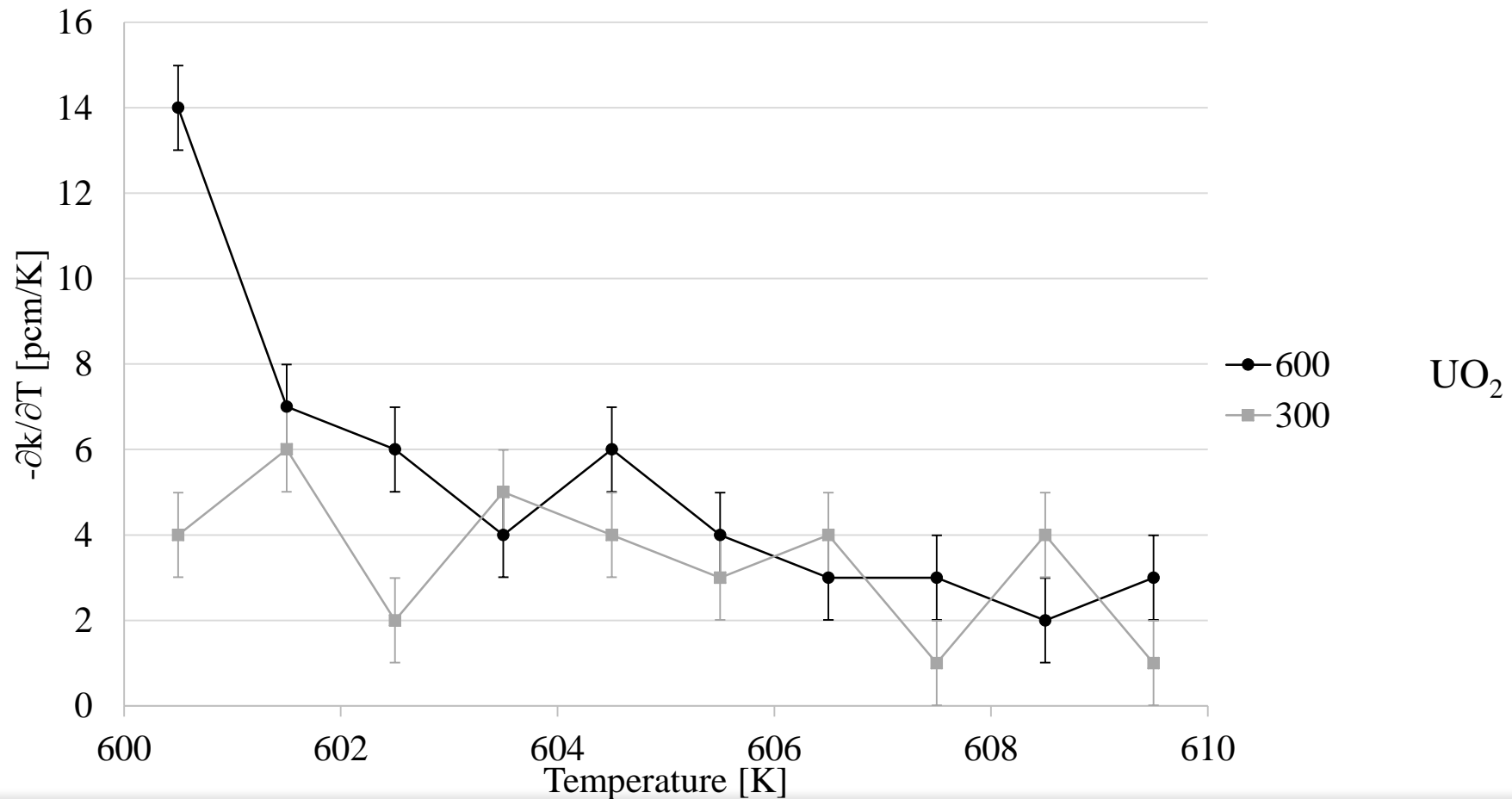
## $U_3Si_2$ Doppler Coefficient



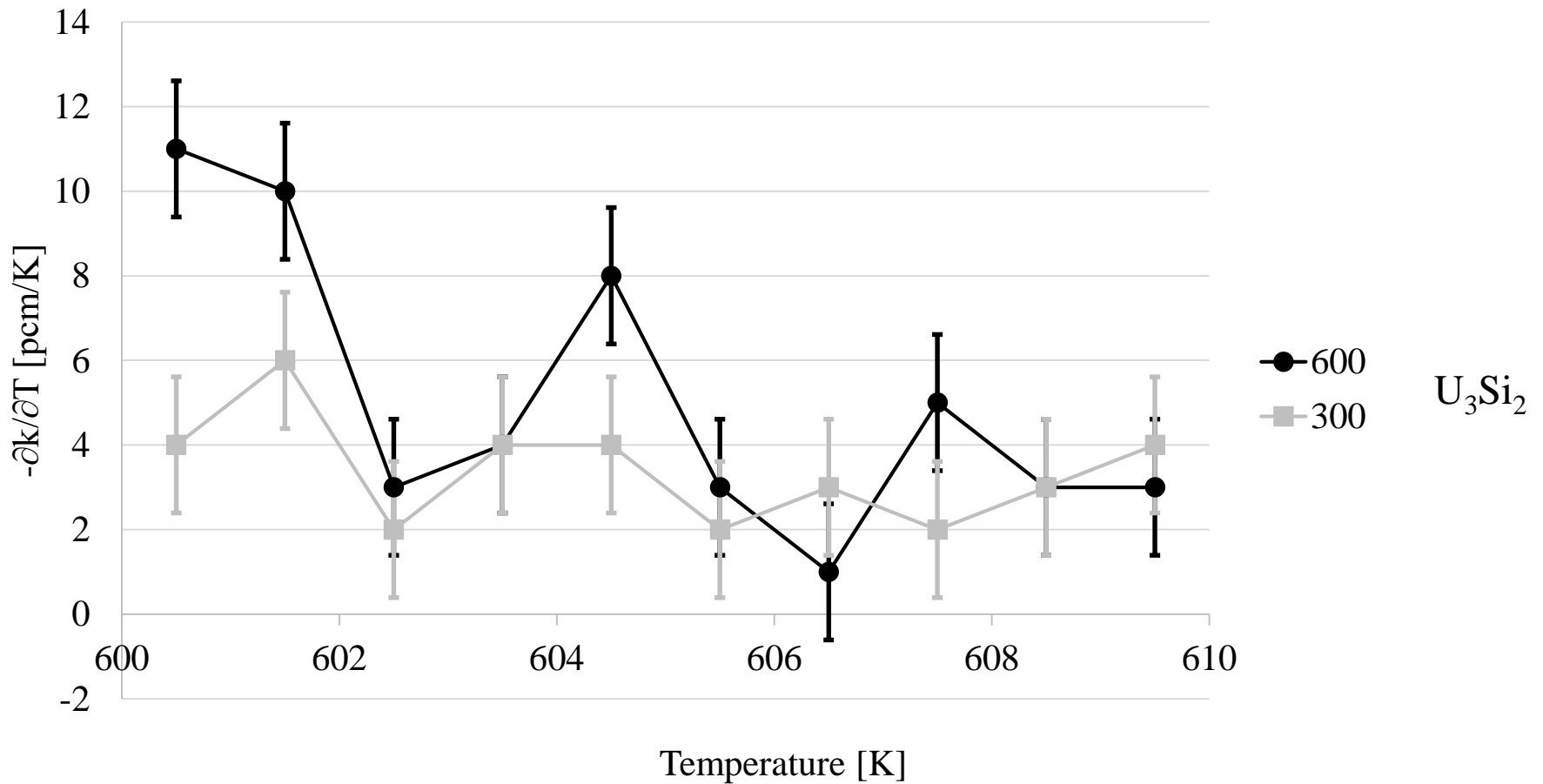
## FHR Doppler Coefficient



# Supplementary



# Supplementary



# Supplementary

