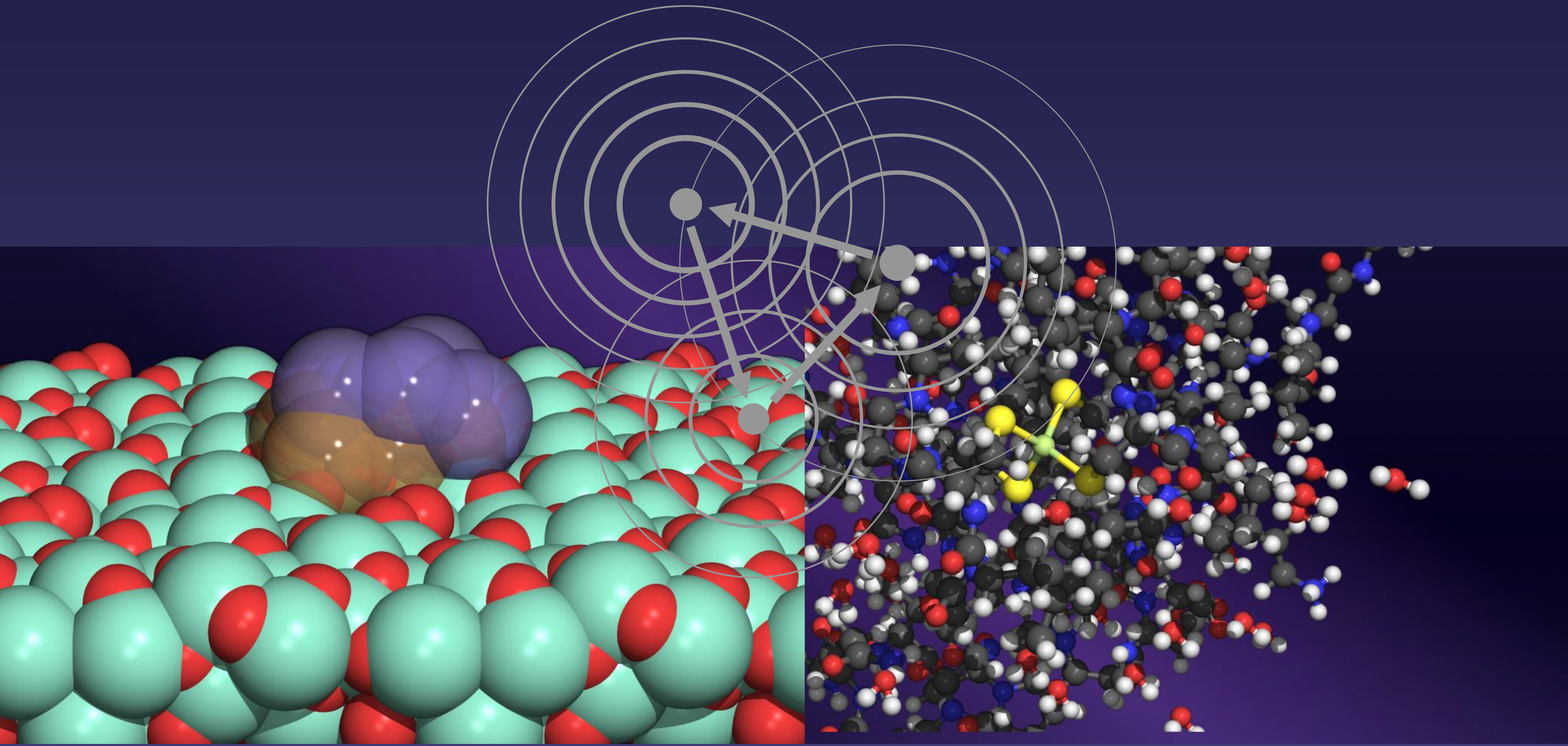
Computational Scattering Science
Argonne National Lab, 2010

Fast and Ultrafast Phenomena



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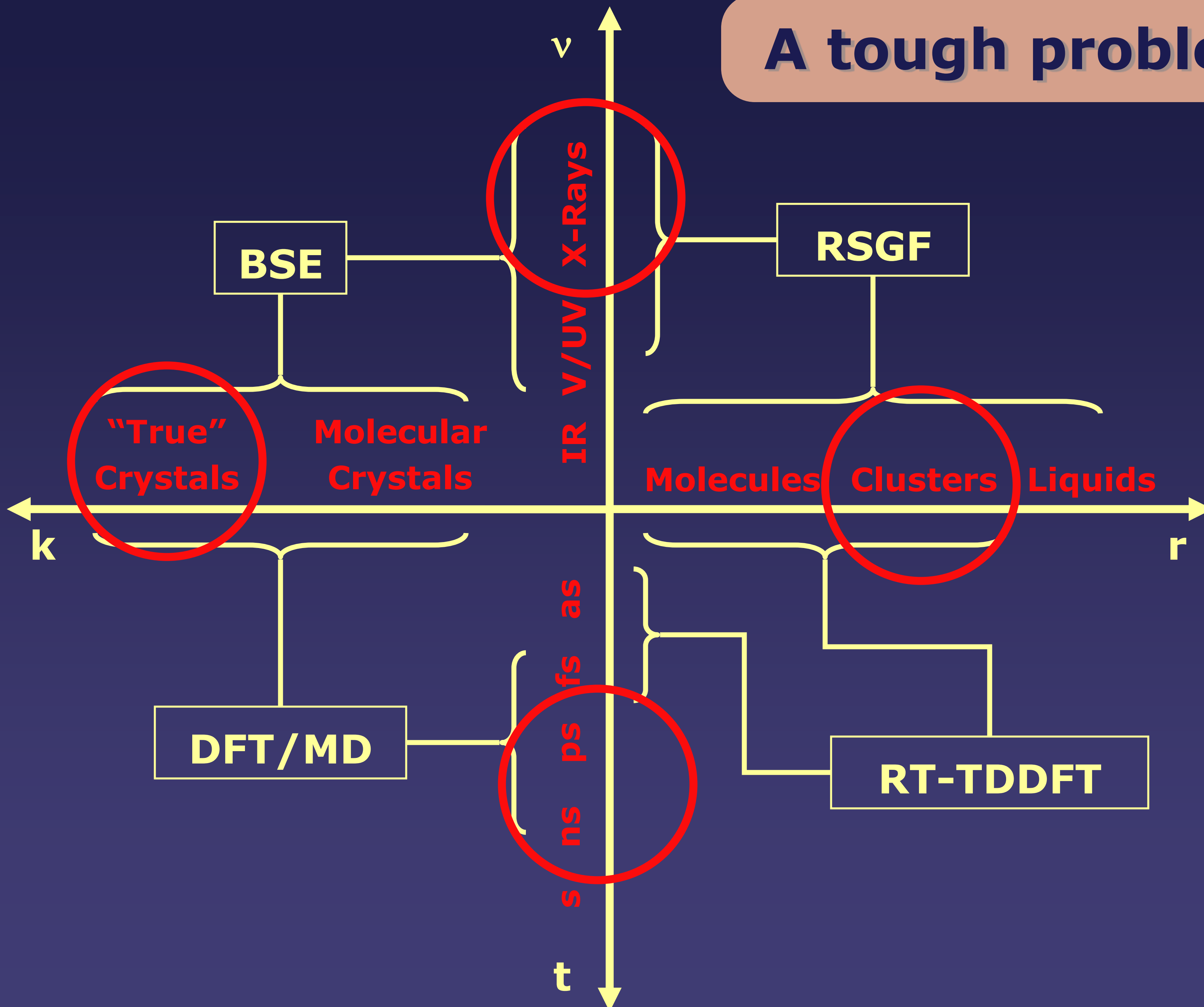
Fast and Ultrafast Phenomena: A special challenge to theory

- Science challenge:
  - From chemical reactions and transient molecular structures, to high-harmonic generation and quantum control, F&UF phenomena encompass a wide variety of problems
  - F&UF phenomena usually involve transient electronic states with a wide range of lifetimes, allowing for different states of equilibrium between the material's dynamical degrees of freedom
- Experimental challenge:
  - New instruments probe regimes that were, until recently, unachievable (More accurate, sensitive and faster, better spatial and temporal resolution)
  - New experimental methods measure properties that still lack computational infrastructure (RXES, RIXS, pump-probe EXAFS and XANES)
- Software challenge:
  - Simulations are currently quite costly, requiring significant phase-space sampling to provide realistic results
  - We are at a juncture were changes in hardware and software landscape are starting to make HPC simulations accessible to "casual" users
  - Currently, most algorithm and software design is characterized by a "piecemeal" approach. We are starting to see some integration of software (driven by necessity)

A tough problem



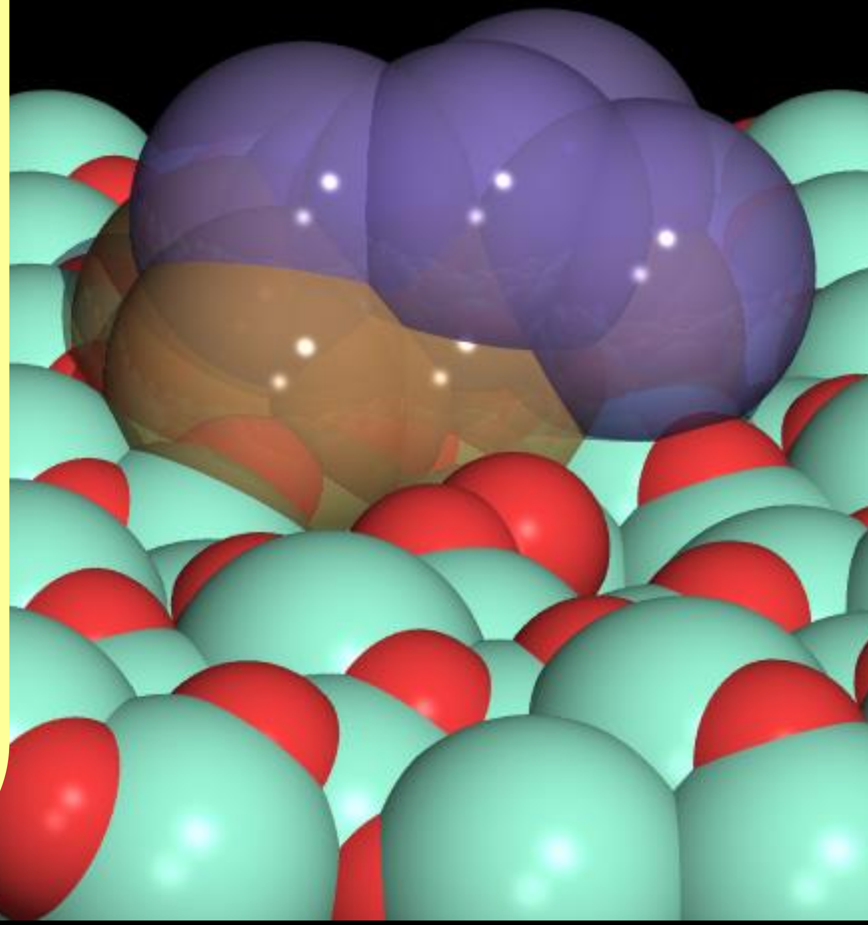
Dynamic Structure in Pt nanoclusters on γ–Al_2O_3

Pt-Pt bond expansion going from He to H_2 atmosphere ❶

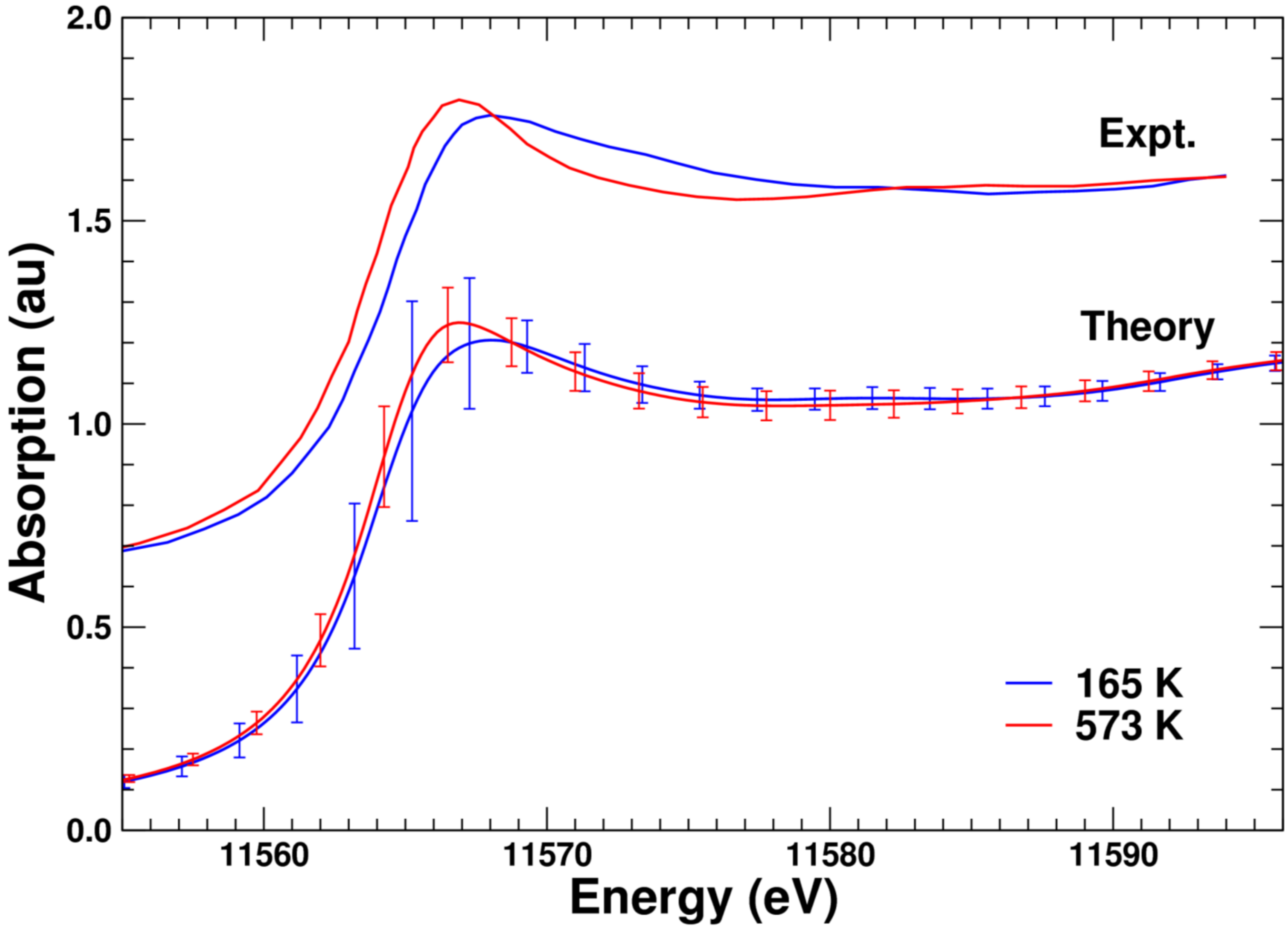
Pt-Pt bond negative thermal expansion ❷

High Pt-Pt disorder ❸

Increased intensity and redshift of XANES with increasing T ❹



④ Increased intensity and redshift at high T



Current state of simulations of F&UF phenomena

- Many different tools are currently being used to study the various incarnations of F&UF phenomena. Can we identify a common simulation infrastructure that encompasses a broad range of them? Do we really want to?
- Would it be preferable to use different approaches for different regimes? If so, how do we bridge the gaps?
- Users are slowly realizing the importance of dynamical sampling. How can we accelerate this? How can we facilitate it in the short term?
- Are there any methodologies that can be easily modified to cover emerging experimental techniques? Which techniques need software development from the ground up?
- How do we reduce the cost of simulation in the short term? Can we take quick advantage of emerging paradigms in hardware and software engineering (Cloud computing, GPU computing, etc)?
- Can we leverage these new paradigms to make better simulations available for “casual” users”?
- There are currently European initiatives for strategic software development (libraries, common data structures, etc). What are the equivalent initiatives on this side of the Atlantic? Should we aim for better pooling of resources?

The next 5 years

- How do we go from one-of-a-kind simulations by expert users, to routine usage of theory by "casual" users and experimentalists?
- What are the common simulation bottlenecks that are hindering this development?
- What are the best ways to integrate the different simulation regimes as well as the experiments? Given the wide range of phenomena involved, how do we bridge the gaps between the fields involved?
- Are there any problems that require specific attention due to specific needs?
- Successful development of research in F&UF phenomena will likely create a deluge of data. How do we plan to handle that data? How can we make it quickly available to facilitate further development?

How do we get there?

- Which algorithms need to be developed or revamped to increase the efficiency of simulations?
- How do we interface the likely different programs that will be needed into a single package that reduces the "idea to results" time?
- Computational Scattering Toolkit?
- How can we make the software widely available and easy to use? Should we offer training opportunities? Outreach?