

Workshop II: Extended Systems and Boundary Conditions

Part of the long program Numerical Algebraic Geometry and Correlated Electrons: Generalized Grassmannians, Response Functions and Excited States

APRIL 19 - 22, 2027

Scientific Overview

This workshop aims to explore the connections and new synergies between numerical algebraic geometry and practical quantum-chemical methods for extended systems. This includes approximate methods for capturing electron correlation such as localized-orbital coupled cluster theory, where a deeper understanding of the underlying mathematical structure promises to gain new insights into the involved approximations and their remaining pitfalls. In the same vein, we aim to extend our previous efforts from workshop I to periodic Hamiltonians and the study of solids and materials. One aspect for the quantum-chemical study of materials as well as extended molecular systems are tensor representations of the wavefunction or electron repulsion integrals and their symmetry properties.

This workshop brings together experts from chemistry, physics, and (numerical) algebraic geometry to explore the structure of the involved tensors and novel ideas for their efficient computation, storage, and usage in electronic structure theory. Finally, many extended systems in chemistry and materials science lend themselves to quantum embedding approaches, where only a subpart is treated at a high level of theory while the rest can be described with more cost-efficient methods. This idea has recently been formulated as a sum-of-squares problem thus offering exciting avenues for algebro-geometric approaches to the characterization and description of (embedded) quantum many-body systems.

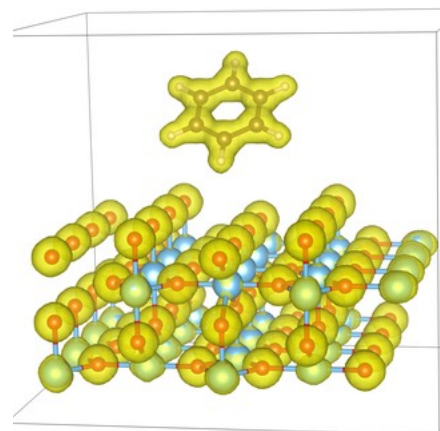
This workshop will include a poster session; a request for posters will be sent to registered participants in advance of the workshop.

This is a Julian Schwinger Workshop on Multiscale Physics, made possible by a gift from the Julian Schwinger Foundation for Physics Research (JSF).

Long Program Schedule

This workshop is part of the long program Numerical Algebraic Geometry and Correlated Electrons: Generalized Grassmannians, Response Functions and Excited States (ALG2027).

- Numerical Algebraic Geometry and Correlated Electrons: Generalized Grassmannians, Response Functions and Excited States - Tutorials: March 9 - 12, 2027
- Workshop I: Numerical Algebraic Geometry: March 30 - April 2, 2027
- **Workshop II: Extended Systems and Boundary Conditions: April 19 - 22, 2027**
- Workshop III: Response Functions, Time-Dependent Properties and Parameterizations: May 3 - 6, 2027
- Workshop IV: Algebraic Varieties and Electronic Structure: May 24 - 27, 2027
- Numerical Algebraic Geometry and Correlated Electrons: Generalized Grassmannians, Response Functions and Excited States - Culmin: June 6 - 11, 2027



Organizers

Volker Blum
Duke University
Marivi Fernandez-Serra
SUNY Stony Brook
Andreas Grüneis
Vienna University of Technology
Joe Kileel
University of Texas at Austin
Todd Martinez
Stanford University
Martin Stoehr
Stanford University

Invited Speakers

Gregory Beylkin (University of Colorado Boulder), **Volker Blum** (Duke University), **George Booth** (King's College London), **Cyrus Dreyer** (Stony Brook University), **Marivi Fernandez-Serra** (SUNY Stony Brook), **Giulia Galli** (University of Chicago & Flatiron Institute), **Andreas Grüneis** (Vienna University of Technology), **Yuehaw Khoo** (University of Chicago), **Joe Kileel** (University of Texas at Austin), **Benjamin Levine** (Stony Brook University), **Lin Lin** (California Institute of Technology), **Michael Lindsey** (University of California, Berkeley (UC Berkeley)), **Jianfeng Lu** (Duke University), **Todd Martinez** (Stanford University), **Sandeep Sharma** (California Institute of Technology), **Martin Stoehr** (Stanford University), **Ed Valeev** (Virginia Tech)



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