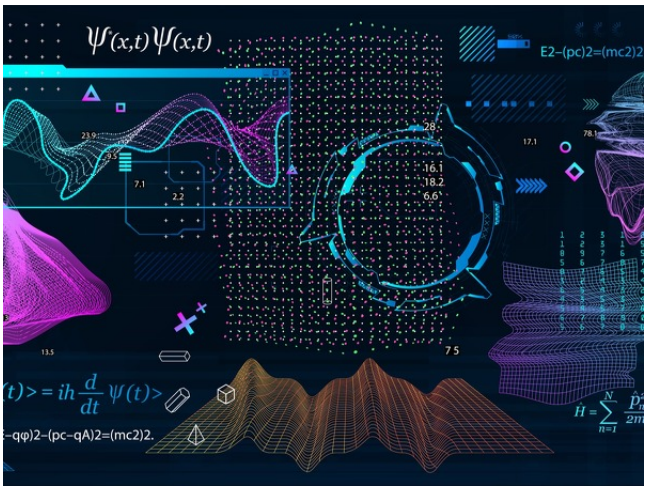
INNOVATION PARTNERSHIPS
UNIVERSITY OF MICHIGAN

GREEN: Simulation of Realistic Materials with Green's Function Methods

TECHNOLOGY NUMBER: 2025-303



Technology ID
2025-303

Category
Software
MOSS - Michigan Open Source Support

Inventor
Emanuel Gull
Sergei Iskakov
Dominika Zgid

Further information
Ashwathi Iyer
ashwathi@umich.edu

View online

OVERVIEW

Comprehensive computational package utilizing Green's function codes for molecular and periodic systems

- Integrated, modular design enhances efficiency, accuracy, and versatility in advanced quantum simulations
- Quantum chemistry, materials science, molecular magnetism, quantum dynamics, and condensed matter research

BACKGROUND

Quantum chemistry and condensed matter physics have long relied on computational approaches to better understand the intricate behaviors of electrons in molecules and solids. Traditional methods—such as density functional theory (DFT)—are powerful for many systems but often fall short in accurately capturing electron correlation effects, especially in strongly correlated materials. Historically, methods extending beyond DFT, such as dynamical mean-field theory (DMFT) and coupled-cluster approaches, have been used, but these can be limited in flexibility, scalability, or modularity. Existing Green's function-based codes are often tailored to specific problems, lack interoperability, or require substantial expertise to adapt for new investigations. With the rise of new materials and the need for rapid exploration of complex phenomena, researchers require integrated, robust tools capable of addressing a broad range of problems, accommodating both existing and novel scientific challenges.

INNOVATION

GREEN introduces a modular, user-friendly computational suite, unifying and extending existing Green's function codes for molecular and periodic systems. By enabling multiple interoperable modules, GREEN provides researchers with the flexibility to analyze weakly and strongly correlated systems, and to develop or integrate new algorithms as scientific needs evolve. The toolbox's technical advances include streamlined post-DFT calculations, advanced handling of quantum dynamics, and the capacity to probe emergent magnetic phases, all within a cohesive platform adaptable to both realistic and model systems. GREEN's versatility makes it suitable for simulating strongly correlated oxide perovskites, studying molecular magnets, and exploring quantum dynamics in small molecules. It empowers users to develop new codes, perform complex simulations, and drive innovation in quantum chemistry, condensed matter, and materials science, ultimately advancing both foundational research and real-world applications.

ADDITIONAL INFORMATION

PROJECT LINKS:

- GREEN Project Website
- GREEN Github

DEPARTMENT/LAB:

- Emanuel Gull, Physics

LICENSE: