Helen Barton Lecture Series in Computational Mathematics

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Friday, October 26, 2018  
Refreshments: 3:30 p.m. in Petty 116  
Talk: 4:00 p.m. in Petty 150  

“Algorithms for Electronic Structure Models”

Abstract: Electronic structure theory has become a workhorse for first principle prediction of properties of chemical and materials systems. In this talk, after introducing the basic elements of electronic structure theory, we will discuss the density fitting procedure for the low-rank approximation of pair products of eigenfunctions of Hamiltonian operator. We will give estimates of the numerical rank of the pair products of eigenfunctions. We will also introduce the interpolative separable density fitting (ISDF) algorithm, which reduces the computational scaling of the low-rank approximation and can be used for efficient algorithms for electronic structure calculations. Based on joint works with Stefan Steinerberger, Kyle Thicke, and Lexing Ying.