

Mathematical Sciences Colloquium

Michigan Technological University

Fisher Hall 127

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1:05 p.m.

Minimization Principles and Computation of Linear Response Eigenvalue Problems

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Abstract: Linear response eigenvalue problems (LREPs) arise from excitation state calculations. In this talk, we will first present theoretical results on minimization principles of LREPs and then discuss how to design conjugate gradient-like algorithms for simultaneously computing the smallest few positive eigenvalues and their associated eigenvectors. Finally, we present numerical results of large-scale LREPs for computing multiple low-lying excitation energies of molecules at both the TDDFT and BSE levels. This is a joint work with Ren-cang Li, Dario Rocca and Giulia Galli.