1116-65-2223 **Ke Yin*** (kyin@math.ucla.edu), 520 Portola Plz, 6363 Math Science, Los Angeles, CA 90095.

Compressed Wannier modes for imperfect crystals and symmetry-adapted Wannier functions. Preliminary report.

This talk introduces two recent development of compressed Wannier modes (CWMs). Wannier functions are some unitary transform of the eigenfunctions of the Hamiltonian with translational symmetry. Inspired by sparse solutions to PDEs, we proposed localized Wannier functions for periodic solids from an L1 regularized energy functional. In the first part of the talk, we describe CWMs for imperfect crystals, where the periodic structures are interrupted by an impurity in one unit cell. Since CWMs are localized in space, the modes that are far away enough from the impurity are not affected. So we keep almost all the modes for the corresponding perfect crystal and only modify those that are affected by the impurity. We describes a systematical way of determining old modes that are needed to modify and replacing them by new modes. In the second part of the talk, we discuss the Wannier functions with symmetry. Since arbitrary unitary transform of a set of Wannier functions is an equivalent representation, not all representations have symmetry. We present a technique to calculate symmetry-adapted compressed Wannier functions, which form the irreducible representation of the symmetry group of the crystal lattice. (Received September 22, 2015)