Density-Functional Partition Theory for Order-N Electonic-Structure and Quantum-Dynamic Computations MORREL COHEN, Department of Chemistry, Princeton University and Department of Physics and Astronomy, Rutgers University, ROBERTO CAR, Department of Chemistry, Princeton University — Large Complex Systems pose a challenge to first-principles electronic-structure and quantum-dynamics computations. Most widely used codes scale as N^3, where N measures the size of the system. In this talk we describe a new order-N scheme based on a new conceptual structure, density-functional partition theory. In partition theory, the system is broken up into mono- or multinuclear parts and its electron density exactly decomposed into contributions from each part. A common partition potential and partition forces acting on each part carry the influence of the rest of the system to that part. A novel functional for the partition potential and a new iteration scheme achieve linear scaling. The scheme will integrate smoothly into the current widely-used Car-Parrinello electronic- and atomic-structure and quantum-dynamics codes.

Morrel Cohen
Department of Chemistry, Princeton University and
Department of Physics and Astronomy, Rutgers University