# Real-Space All-electron Band Structure Calculations

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We are presenting an all-electron numerical framework for band structure calculations. A 3D finite element mesh is used to discretize the DFT/Kohn-Sham problem in real space using full ionic local potential (without introducing pseudopotentials). The mathematical model allows flexibility for addressing various combinations of Bloch and Dirichlet boundary conditions for low-dimensional nanostructures, and the resulting large-scale eigenvalue problems are solved using the FEAST solver [1]. The FEAST algorithm [2] offers many important and unique capabilities for achieving accuracy, robustness, high-performance and scalability on parallel computing architectures. At first, the algorithm can operate in parallel to obtain core and valence electrons independently spanning different energy ranges. Secondly, solving the original eigenvalue problem within a given energy range (i.e. search interval) is mainly reformulated into solving a set of well-defined independent linear systems along a complex energy contour. Additionally, a muffin-tin domain decomposition can be used directly to solve the resulting linear systems [3] without the need to reformulate the original eigenvalue problem into a non-linear one (as it the case using the APW technique [4]). The complexity of numerical framework scales linearly with the number of atoms, and it is flexible to address arbitrary impurities, defects and roughness. Numerical simulation results using DFT/LDA are first presented for polyparaphenylene (PPP) [5], which are in strong agreement with [6]. Band structure calculations of other graphene nanoribbon configurations (n-AGNR) and carbon nanotubes (n-n CNT) will then also be presented and discussed.

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