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Accelerating large scale Kohn-Sham density functional theory calculations with semi-local functionals and hybrid functionals[1]

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The computational cost of standard Kohn-Sham density functional theory (KSDFT) calculations scale cubically with respect to the system size, which limits its use in large scale applications. In recent years, we have developed an alternative procedure called the pole expansion and selected inversion (PEXSI) method [1-2]. The PEXSI method solves KSDFT without solving any eigenvalue and eigenvector, and directly evaluates physical quantities including electron density, energy, atomic force, density of states, and local density of states. The overall algorithm scales as at most quadratically for all materials including insulators, semiconductors and the difficult metallic systems. The PEXSI method can be efficiently parallelized over 10,000 - 100,000 processors on high performance machines. The PEXSI method has been integrated into a number of community electronic structure software packages such as ATK, BigDFT, CP2K, DGDFT, FHI-aims and SIESTA, and has been used in a number of applications with 2D materials beyond 10,000 atoms [3]. The PEXSI method works for LDA, GGA and meta-GGA functionals. The mathematical structure for hybrid functional KSDFT calculations is significantly different. I will also discuss recent progress on using adaptive compressed exchange method for accelerating hybrid functional calculations [4]. References: [1] L. Lin, J. Lu, L. Ying, R. Car and W. E, Fast algorithm for extracting the diagonal of the inverse matrix with application to the electronic structure analysis of metallic systems, Commun. Math. Sci. 7, 755, 2009 [2] L. Lin, M. Chen, C. Yang and L. He, Accelerating atomic orbital-based electronic structure calculation via pole Expansion and selected inversion, J. Phys. Condens. Matter 25, 295501, 2013 [3] W. Hu, L. Lin, C. Yang, J. Dai and J. Yang, Edge-modified phosphorene nanoflake heterojunctions as highly efficient solar cells, Nano Lett. 16 1675, 2016 [4] L. Lin, Adaptively compressed exchange operator, J. Chem. Theory Comput. 12, 2242, 2016