

# **ACRES: an efficient method for first-principles electronic structure calculations of complex systems**

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We present our new implementation of the Adaptive Coordinate Real-space Electronic Structure (ACRES)[1] method for studying the atomic and electronic structure of infinite periodic as well as finite systems, based on density functional theory. This improved version aims at making the method widely applicable and efficient, using high-performance fortran on parallel architectures. We review the new developments that lead to enhanced performance, and present the scaling of various parts of an ACRES calculation. We illustrate the application of ACRES to the study of elemental crystalline solids (alkali metals, group II A metals, sp-electron metals, d-electron magnetic and non-magnetic metals, semiconductors and insulators), and a few molecules composed of atoms in the first row of the periodic table, as well as to the investigation of complex crystalline material properties, such as the band structure of blue bronze, a quasi one-dimensional conductor, and the structure of the “TON” zeolite, a complex crystal composed of Si-O tetrahedra and large pores, which represents a molecular sieve.

## **References**

- [1] N. A. Modine, G. Zumbach, and E. Kaxiras, Phys. Rev. B **55**, 10289 (1997).