THE SIESTA METHOD AND SOME RECENT DEVELOPMENTS

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The suitability of local functions as basis sets for linear−scaling electronic structure methods allowed the development of linear−scaling DFT methods based on them. The Siesta method is based on strictly localised atomic orbitals and represents a quite widely used alternative to more traditional electronic−structure techniques. The fundaments of the methodology will be reviewed, including the utilised basis sets, their performance and evolution, as well as some examples of applicability. Two recent methodological developments will be presented as well, both related to atomic motions: efficient structural relaxations and calculation of free energies.