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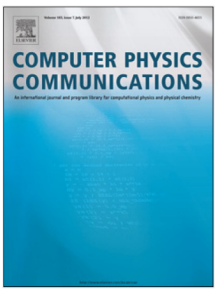

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Compression of Wannier functions into Gaussian-type orbitals

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Abstract

We propose a greedy algorithm for the compression of Wannier functions into Gaussian-polynomials orbitals. The so-obtained compressed Wannier functions can be stored in a very compact form, and can be used to efficiently parameterize effective tight-binding Hamiltonians for multilayer 2D materials for instance. The compression method preserves the symmetries (if any) of the original Wannier function. We provide algorithmic details, and illustrate the performance of our implementation on several examples, including graphene, hexagonal boron-nitride, single-layer FeSe, and bulk silicon in the diamond cubic structure.

1 Introduction

Since their introduction in 1937 [32], Wannier functions have become a widely used computational tool in solid state physics and materials science. Theses functions provide insights on chemical bonding in crystalline material [14], they play an essential role in the modern theory of polarization [10], they can be used to parametrize tight-binding Hamiltonians for the calculation of electronic properties [8], and are useful in several other applications [14].

Maximally localized Wannier functions (MLWFs) were introduced by Marzari and Vanderbilt [15] and are obtained by minimizing some spread functional [15, 26, 14]. Several algorithms for generating MLWFs are implemented in the Wannier90 computer program [18]. In the general case, MLWFs obtained by the standard Marzari-Vanderbilt procedure are not centered at high-symmetry points of the crystal (typically atoms or centers of chemical bonds), and do not fulfill any symmetry properties [26, 30], which complicates their physical interpretation. Symmetry-adapted Wannier functions (SAWFs) are centered at high-symmetry points and are associated with irreducible representations of a non-trivial subgroup of the space group of the crystal (precise definitions are given in Appendix). They are the solid-state counterparts of symmetry-adapted molecular orbitals [13] that are fruitfully used in quantum chemistry. SAWFs were investigated in [5, 11, 31, 12, 27, 6, 25, 24, 21, 3] from both the theoretical and the numerical point of view. An algorithm for generating maximally-localized SAWFs was