Maximally Localized Wannier Functions: Concepts, Applications, and Beyond

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ABSTRACT

Maximally localized Wannier functions provide a representation of the electronic structure in terms of spatially localized functions which is particularly insightful. Since their introduction, these functions have found numerous applications in solid-state theory and in *ab-initio* simulation, in physics and in chemistry. More recently, these functions have grown into a methodological tool for the study of polarization, magnetism, strongly-correlated electrons, transport, and large-scale electronic systems. This workshop provides a forum where these novel ideas are confronted and shared across research fields.
SCIENTIFIC SUMMARY (1000 words)

The electronic structure of periodic systems is usually described in terms of the energy eigenfunctions, the Bloch functions, which are also eigenstates of the translation operator. However, these functions are spatially delocalized and offer a description which is not very intuitive. An alternative description of the electronic structure is provided by Maximally Localized Wannier Functions (MLWFs), which favor a representation of the electronic structure in terms of functions localized in real space [1,2]. These functions are obtained by unitary transformation from the energy eigenfunctions and therefore provide a fully equivalent description. Through their center, their extension and their shape, MLWFs provide a description of the electronic structure which is physically insightful. The electron orbitals can be visualized and located with respect to the positions of the atoms. Early investigations on complex crystals [2] and on disordered solids [3] and liquids [4] immediately illustrated the strength of this new concept. Essentially, a MLWF provides information on the local electronic structure in a straightforward and compact form.

Maximally localized Wannier functions are experiencing an increasing success as a monitoring tool of the electronic structure within both the electronic structure [5-9] and ab-initio molecular dynamics communities [10-12]. However, more recently, the particular properties of MLWFs have also attracted interest as a primary methodological tool within more complex theoretical developments. The most interesting aspect of MLWFs is that they allow a decomposition of the electronic structure in local components [1,2]. This property naturally allows one to locally monitor the response of the electronic structure when the investigated system is perturbed, either by the application of external (electric or magnetic) fields or by structural modification. In the study of the polarization, the usefulness of MLWFs is further enhanced by the fact that the displacement of their centers naturally connects with the modern definition of the polarization [1,2]. Hence MLWFs have become the method of choice to investigate the dielectric response in insulator-insulator [13-16] or insulator-metal interfaces [17]. Similarly, MLWFs have shown their usefulness in the study of the response of the electronic structure to a magnetic field [18-20]. These functions have been used in the calculation of NMR shifts [18], but have also turned out to be valuable in establishing the correct definition of the orbital magnetization in periodic systems [19,20]. Recent work on the interpretation of photoemission shifts at semiconductor surfaces and interfaces relies on MLWFs to highlight the role of strain fields [21].

Another exploited property of a set of MLWFs is that they constitute a complete basis set for the occupied states in which hierarchy can be established on the basis of distance to a particular point in space. This property is particularly useful for the introduction of approximations in which role of the local electronic structure is prioritized. Such basis functions have found a natural application in the development of methodologies for large-scale electronic calculations [22,23]. Recent developments also concern the research area of strongly correlated electrons, where MLWFs have recently been introduced as preferred functions for describing the local correlation [24-31].

Maximally localized Wannier functions have also found application in the construction of simplified Hamiltonians for multi-scale approaches. In this case, one uses the property that MLWFs can represent a particular energy window. This is straightforward when the relevant electronic bands are well separated from the other ones, but recent developments have extended such applications also to coupled bands introducing purposely designed
disentanglement procedures [32-35]. In particular, these methodological developments are at the basis of several successful applications in the context of transport in nano-sized structures [36-38].

Although most of the early applications of MLWFs were to insulating systems, very recently the usefulness of partially-occupied MLWFs as fast and accurate interpolators for describing Fermi-surface properties of metals has been explored. For example, this has been used to reduce dramatically the computational load needed to evaluate properties such as the anomalous Hall effect of ferromagnets [39] and the electron-phonon coupling [40]. A further recent extension has shown that generalized Wannier functions can be constructed which show small spreads both in space and in energy [41].

The raise of interest in MLWFs has also prompted theoretical work in order to complete the characterization of these functions. Very recent work has been able to demonstrate the exponential nature of the localization [42], extending to three dimensions previous work for one dimension [43]. Furthermore, the real nature of MLWFs, empirically observed in many applications, could be formally demonstrated [42]. The wide-spread use of MLWFs in the ab initio simulation community has also led to the development of molecular dynamics integrators which preserve the localization properties during the course of the evolution [44-46].

A computer module for the generation of MLWFs is freely available [47] and facilitates their wide-spread use across the electronic-structure community. The success of MLWFs has brought several major software packages, such as DACAPO, CPMD and QUANTUM-ESPRESSO, to offer to their users a module for their generation. From the technical point of view, there have been important evolutions in the algorithms that are used to generate MLWFs [48-51].

Finally, it should be mentioned that the concept of MLWF has acquired generality giving rise to applications which extend beyond the description of the electronic structure. For instance, the concept has been used in the context of photonic crystals [52] and recent work shows how generalized Wannier functions can be used to study phonon Hamiltonians [41,40].

As clearly illustrated by this evolution, the use of MLWFs is rapidly expanding across diverse research areas. One of the primary aims of the present workshop is to bring together the major players in these different disciplines in order to share their experiences. These will include researchers in the electronic structure and ab initio simulation community, in physics and in chemistry. Researchers that are primarily interested in new developments and researchers that are more concerned with practical applications will be both represented. While the research areas are diverse, the optimal integration of MLWFs in broader schemes necessarily will face difficulties which are to a large extent common to all concerned research areas. The workshop represents a forum where researchers from various fields meet to expose their views, discuss their ideas, and confront their solutions. Furthermore the interaction between development and application will be beneficial to both parties leading to more focused developments on the one side, and to richer applications on the other.

The planned workshop is the very first one of this nature. The impact of the workshop is expected to be twofold. First, at this time it is not clear whether all the major researchers that have been identified in this proposal are fully aware of all the developments that are occurring
in parallel in other research areas. The workshop will therefore contribute in removing potential communication barriers. This will be beneficial to several research fields. Second, the workshop will promote the interaction between development and application. Eventually this will lead to the optimal exploitation of the concept of MLWFs in various contexts.

**FORMAT**

We are planning a three-day workshop with 28 participants, to be held at CECAM in Lyon. The workshop will cover all the main research areas in which maximally localized Wannier functions are currently having impact. We are planning to have 9 to 10 talks per day. The workshop will start with an overview talk that reviews the field at large, both the history and the state of the art, open problems, etc. David Vanderbilt kindly accepted to give such an opening talk. The other talks will then be grouped according to the following themes:

(i) **GENERAL THEORY AND ALGORITHMS**,  
(ii) **POLARIZATION**,  
(iii) **MAGNETISM AND SPIN-ORBIT EFFECTS**,  
(iv) **STRONGLY CORRELATED ELECTRONS**,  
(v) **TRANSPORT**,  
(vi) **LARGE SCALE ELECTRONIC-STRUCTURE CALCULATIONS**, and  
(vii) **APPLICATIONS**.

Each participant will be allotted 30 minutes and an indicative time schedule will be set up, in which the scheduled discussion time is approximately equivalent as the presentation time. Rather than enforcing a rigid schedule, the chairman of each session will be allowed to freely manage the discussion time available to his session following the interest of the audience.

**PREFERRED DATES**

27.06.2007 - 29.06.2007

**BUDGET**

- Living expenses for a three-day workshop with 28 participants  
  28 people x 3 days x 90 EUR = 7560 EUR
- Traveling expenses of organizers  
  Marzari Boston (400 EUR), Sousa San Francisco (700 EUR)  
  Pasquarello Lausanne (100 EUR)  
  1200 EUR
- Traveling expenses 12 participants (non-organizers) from USA  
  12 people x 300 EUR = 3600 EUR
- social dinner  
  28 people x 40 EUR = 1120 EUR
- coffee breaks  
  6 breaks x 28 people x 2 EUR = 336 EUR

**TOTAL**  
13816 EUR
SUPPORT

We are submitting this application, simultaneously to CECAM and ESF (Psi-k programme), seeking financial support for a joint CECAM/Psi-k workshop. The research area covered by our proposal is expanding rapidly both in Europe and in the United States, as appears clearly from the list of participants that we are proposing. In order to ensure that the main players in the field are optimally represented, we are therefore seeking funding from ESF through the Psi-k programme, in addition to the budget allocated by CECAM for a regular three-day workshop. This workshop proposal, which intends to bring together researchers from simulation and electronic structure, appears particularly suited to be announced as a joint CECAM-Psi-k workshop. We will also encourage the young participants from overseas to seek for additional funding through the NSF.

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Five most relevant papers of Nicola Marzari during the last five years

1) M. Cococcioni, F. Mauri, G. Ceder, and N. Marzari,
   Electronic-enthalpy functional for finite systems under pressure,
2) Y.-S. Lee, M. Buongiorno Nardelli, and N. Marzari,
   Electronic-structure and quantum conductance of nanostructures from maximally-localized
   Wannier functions: the case of functionalized nanotubes,
   PHYSICAL REVIEW LETTERS 95, 076804 (2005).
3) B. Kozinski and N. Marzari,
   Static dielectric properties of carbon nanotubes from first principles,
4) H.-L. Sit, M. Cococcioni, and N. Marzari,
   Realistic, quantitative descriptions of electron-transfer reactions: diabatic surfaces
   from first-principles molecular dynamics,
   PHYSICAL REVIEW LETTERS 97, 028303 (2006).
5) H. J. Kulik, M. Cococcioni, D. A. Scherlis, and N. Marzari,
   Density-functional theory in transition-metal chemistry: A self-consistent
   Hubbard U approach,
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Five most relevant papers of Alfredo Pasquarello during the last five years

1) Pasquarello A, Petri I, Salmon PS, Parisel O, Car R, Toth E, Powell DH, Fischer HE, Helm L, Merbach AE,
   First solvation shell of the Cu(II) aqua ion: Evidence for fivelfold coordination,
2) Umari P, Pasquarello A,
   Ab initio molecular dynamics in a finite homogeneous electric field,
   PHYSICAL REVIEW LETTERS 89, 157602 (2002).
3) Bongiorno A, Pasquarello A,
   Oxygen diffusion through the disordered oxide network during silicon oxidation,
   PHYSICAL REVIEW LETTERS 88, 125901 (2002).
4) Giustino F, Umari P, Pasquarello A,
   Dielectric discontinuity at interfaces in the atomic-scale limit:
   Permittivity of ultrathin oxide films on silicon,
   PHYSICAL REVIEW LETTERS 91, 267601 (2003).
5) Bongiorno A, Pasquarello A, Hybertsen MS, Feldman LC,
   Transition structure at the Si(100)-SiO2 interface,
   PHYSICAL REVIEW LETTERS 90, 186101 (2003).

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Five most relevant papers of Ivo Souza during the last five years

1) Ivo Souza, Nicola Marzari, and David Vanderbilt,
   Maximally-localized Wannier functions for entangled energy bands,
   PHYSICAL REVIEW B 65, 035109 (2002)
2) Ivo Souza, Jorge Iniguez, and David Vanderbilt,
   First-Principles Approach to Insulators in Finite Electric Fields,
   PHYSICAL REVIEW LETTERS, 89, 117602 (2002).
3) Ivo Souza, Jorge Iniguez, and David Vanderbilt,
   Dynamics of Berry-phase polarization in time-dependent electric fields,
   PHYSICAL REVIEW B 69, 085106 (2004).
4) Xinjie Wang, Jonathan R. Yates, Ivo Souza, and David Vanderbilt,
Ab-initio calculation of the anomalous Hall conductivity by Wannier Interpolation, 
(submitted to PHYSICAL REVIEW B, preprint cond-mat/0608257).
5) Feliciano Giustino, Jonathan R. Yates, Ivo Souza, Marvin L. Cohen, and Steven G. Louie,
Electron-Phonon Interaction via Electronic and Lattice Wannier functions: 
Superconductivity in Boron-Doped Diamond Reexamined, 
(submitted to PHYSICAL REVIEW LETTERS).

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diagonalization algorithm

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