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First Principles Approaches to Spectroscopic Properties of Complex Materials

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Complexity has become a current keyword with several different meanings. Referred to materials, complexity can stay for the coexistence of different, possibly conflicting properties, such as band gap and conductivity, magnetism or ferroelectricity and superconductivity, etc. Multifunctionality is a practical consequence of such a coexistence. Irreducibility, non-extensivity and emerging properties are all aspects of complexity, whose description and prediction severely challenge first-principle methods. The exponential growth of computer power, and the simultanoeus descent of device technology to the nanoscale have allowed quantum theory and experiment to overlap, so that predicting and optimizing real nanostructures by means of quantum theory and computation is becoming current practice.

The density functional theorem belongs to the small family of fundamental exact theories of physics, but for each of them there is an ingredient concerning the complexity of nature which we need to know as well as possible. For Maxwell equations it is the electromagnetic response function of the system; for DFT the energy functional, which in turn enables us to determine the e-m response. The climb to complex materials is parallel to that of *ab initio* theory of e-m response functions and related spectroscopies: new classes of materials have stimulated a progress in DFT-based *ab initio* methods, and this progress has often led to conceive new materials with multiple functions at the nanoscale. Today this comparably fast parallel climbing is enabled by a close synergy between experiment and theory, *i.e.*, by large-scale research networks.

The editors present the book as an overview of state-of-the-art methods in computational spectroscopy, a guide to approximations and how to expand DFT predicting power, thus providing a scenario of expected evolution. Actually the editors have made an excellent job in planning and organizing the book in a way that each chapter can be viewed from the point of view of paradigmatic materials or from that of benchmark methods. In Chapt. 1 (Pastore, Selloni, Fantacci, de Angelis) time-dependent DFT is confronted with dye-sensitized titanium dioxide for solar cells. For the transition-metal oxides Bendavid and Carter (Chapt. 2) expose the DFT integrated by the GW approximation, and eventually by the Bethe-Salpeter approach for an accurate description of neutral excitations. Bruneval and Gatti (Chapt. 3) illustrate the power of the quasiparticle self-consistent GW method for band and strongly correlated insulators.

Gas-phase valence-electron photoemission spectroscopy of complex organic molecules like NTCDA, nicely illustrated by Reut Baer's lovely drawing, can now profit of quite accurate TDDFT description and predictions, as well explained by Kronik and Kümmel (Chapt. 4). The concept of orbital-density functionals fulfilling Koopmans theorem solves problems of quasi-particles levels and computational photoemission. Dabo, Ferretti and Marzari demonstrate that (Chapt. 5) by comparing computed and experimental ionization and orbital energies of several elements up to Kr, and the electron affinities of various organic molecules and fullerenes. A central chapter of the book, for position and significance, is that by Sharma, Dewhurst and EKU Gross introducing TDDFT with an outline of the Runge-Gross theorem and illustration of a basic ingredient – the nanoquanta kernel – allowing for a good description of excitonic physics in extended systems like Si crystals and large band-gap insulators such as diamond, LiF and Ar. In Chapt. 7 (C. Friedrich *et al.*) magnetism comes about explicitly with spin elementary excitations in solids calculated with many-body perturbation theory, notably the FLAPW method.

Silke Biermann (Chapt. 8) exposes the progress in dynamical mean-field theory (DMFT) for correlated materials like manganese, titanates and iridates, and rare-earth pigments, and the strategies to derive Hubbard interaction from LDA-DMFT. Hopjan and Verdozzi open a window of the problem of strongly correlated materials under non-equilibrium conditions, as occurring in time-dependent, actually ultrafast femto- and atto-second spectroscopies, which have known a tremendous progress in recent times. The corresponding progress in the use of non-equilibrium Green's functions and TDDFT is the subject of the last chapter of the book. The editors add a final important and useful note on the Bethe-Salpeter equation, considering that its notion and power have been assumed in some chapters as well known. Besides the choice of the subjects, a special merit of the editors and of this collection of articles is the size and completeness of the chapters, each one enriched by monumental bibliographies, which makes this book extremely useful.

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