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# UNDERSTAND, PREDICT, AND DESIGN

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Electronic-structure approaches are changing dramatically the way much theoretical and computational research is done. This success derives from the ability to characterize from first-principles many material properties with an accuracy that complements or even augments experimental observations. This accuracy can extend beyond the properties for which a real-life experiment is either feasible or just cost-effective, and it is based on our ability to compute and understand the quantum-mechanical behavior of interacting electrons and nuclei. Density-functional theory, for which the Nobel prize in chemistry was awarded in 1998, has been instrumental to this success, together with the availability of computers that are now routinely able to deal with the complexity of realistic problems. The extent of such revolution should not be underestimated, notwithstanding the many algorithmic and theoretical bottlenecks that await resolution, and the existence of hard problems rarely amenable to direct simulations. Since *ab-initio* methods combine fundamental predictive power with atomic resolution, they provide a quantitatively-accurate first step in the study and characterization of new materials, and the ability to describe with unprecedented control molecular architectures exactly at those scales (hundreds to thousands of atoms) where some of the most promising and undiscovered properties are to be engineered. In the current effort to control and design the properties of novel molecules, materials, and devices, first-principles approaches constitute thus a unique and very powerful instrument. Complementary strategies emerge:

- *Insight:* First-principles simulations provide a unique connection between microscopic and macroscopic properties. When partnered with experimental tools – from spectroscopies to microscopies – they can deliver unique insight and understanding on the detailed arrangements of atoms



*S. Yip (ed.),*
*Handbook of Materials Modeling,* 9–11.

and molecules, and on their relation to the observed phenomena. *Gedanken* computational experiments can be used to prove or probe cause-effect relationships in ways that are different, and novel, compared with our established approaches.

- *Control:* Microscopic simulations provide an unprecedented degree of control on the systems studied. While macroscopic behavior often emerges from complexity – thus explaining all the ongoing efforts in overcoming the time- and length-scale limitations – fundamental understanding needs to be built from the bottom-up, under the carefully controlled condition of a computational experiment. Simulations can offer early and accurate insights on complex materials that are challenging to control or characterize.
- *Design:* Quantitatively accurate predictions of materials' properties provide us with an unprecedented freedom, a "magic wand" that can be used with ingenuity to try and engineer novel material properties. Intuitions can often be rapidly validated, shifting and focusing appropriately the synthetic challenge to the later stages, once a promising class of materials has been identified.
- *Optimization:* Finally, the systematic exploration of material properties inside or across different classes of materials can highlight the potential for absolute or differential improvements. Stochastic techniques such as data mining and optimization then identify the most promising candidates, narrowing down the field of structures to be targeted in real-life testing.

While the extent and scope of this emerging discipline are nothing short of revolutionary, researchers in the field face key challenges that are worth remembering: achieving thermodynamical accuracy, bridging length-scales, and overcoming time-scales limitations. It is unlikely that an overarching solution to these problems will appear, and much of the art of modeling goes into solving these challenges for the problem at hand. It is nevertheless important to remark the role of correlations: whenever the typical correlation lengths become smaller then the size of the simulation box (e.g., for a liquid studied in periodic-boundary conditions), the system studied becomes virtually infinite, and the finite-size bias irrelevant.

The articles presented in this volume offer a glimpse on the panorama of electronic-structure modeling; in such distinguished company, it would be inappropriate for me to condense such diverse and exciting contributions into a few sentences. I will leave the science to the authors, and conclude with a few statements on future developments.

The continuous improvement in the price vs. performance ratio for commodity CPUs is now widely apparent. Whereas computational resources seem never enough, and the desire of a longer and bigger simulation is always looming, we are now in the position where even a single desktop is sufficient to

sustain research of world-class quality (of course, human resources are even more precious, and human ingenuity can be sometimes light-heartedly traded for sheer computational power).

This availability of computer power is now combined with the availability of state-of-the-art computer packages – some of them freely distributed and developed under a shared-community, public-license model akin to that, e.g., of Linux. The net result has been that "computational laboratories" around the world have been increasing in capability with a speed comparable to Moore's law, their hardware and software infrastructures replicated almost at the flick of a switch. Some conclusions can be attempted:

- The geographic distribution of researchers in this field might change significantly. World-class science can now be done inexpensively and extensively, and knowhow and human resources become almost exclusively the most precious commodities.
- Publicly available electronic structure packages take the role of internationally shared infrastructures; in perfect analogy with the way brick-and-mortar facilities (such as synchrotrons) serve many groups in different countries. It could even be argued that investment in "computational infrastructures" (electronic-structure packages) can have comparable benefits, and a remarkable cost structure.
- While these technologies become faster, more robust, and prettier, they also become more and more complex, often requiring years of training to be mastered – content and expertise could also be developed and freely shared following similar public-license models.

The last point brings us back to one of the greatest challenges, and one for which we hope this Handbook will bring a positive contribution: how to avoid trading contents for form, critical thinking for indiscriminate simulations. In T.S. Eliot's words: "The last temptation is the greatest treason: To do the right deed for the wrong reason."