Boosting materials modelling

Basic hurdles in materials modelling, such as access to experimental raw data, thwart fast progress. Governmental and grass-roots initiatives have stepped up to help overcome current limitations.

Theoretical and computational modelling is omnipresent in materials research. The insight provided by *ab initio* and other modelling approaches into the properties of materials is key to both basic and industry-oriented research; this is reflected in, for instance, the increasing number of articles and international patents making use of density functional theory (DFT) calculations — one of the most widely used modelling methods in materials science (Fig. 1).

Modelling can significantly assist in reducing the current timescales needed for the translation of basic research in advanced materials to manufacturing. Different governmental initiatives aimed at improving current modelling capabilities in order to increase industrial competitiveness have therefore been launched. In 2011, the US President Barack Obama announced the Materials Genome Initiative (MGI) promising a renaissance of the American manufacturing industry[1,2]. The main idea behind MGI, which has received over US$250 million from the federal government since it was launched, is to coordinate research activity in materials science with scientific and industrial policies, as well as with financial and infrastructural resources, to speed up the process of discovering and manufacturing materials. Within this framework, different programmes relying on the synergetic collaboration between materials scientists, with experimental and theoretical expertise, and computer scientists have been initiated. A successful example is the so-called Materials Project, which aims to expedite the design of new materials by offering an online open database — currently comprising DFT simulations of over 66,000 compounds and their properties — and analysis tools for interactive exploration and data mining; new battery materials, transparent conducting oxides and thermoelectric materials have already been identified through this initiative[3].

The European Commission also recognizes that materials modelling is key to shorten timescales from basic research to manufacturing of advanced materials[4], which represent one of the key enabling technologies, together with nanotechnology, biotechnology and advanced manufacturing and processing, for the modernization

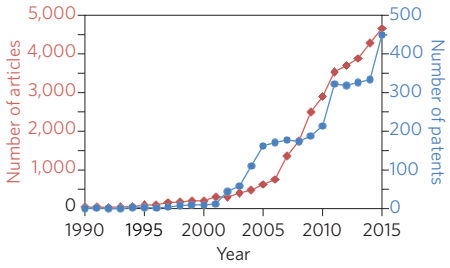

Figure 1 | Number of articles and patents in materials science including the term "density functional theory" published per year during the past 25 years. Article data taken from Scopus, patent data taken from Patentscope.

of the EU industry and the development of advanced and sustainable economies[5]. These technologies constitute one of the pillars of the EU Horizon 2020 research and innovation programme[6]. Europe has a large potential in terms of manpower; about 11,000 researchers working in materials modelling — half of the worldwide *ab initio* community — are based in European countries[7].

In addition to these governmental programmes, bottom-up initiatives have also been developed. For example, the Psi-k community[8] is a Europe-based worldwide community network formed by more than 2,000 scientists, whose aim is to develop first-principles computational materials science — including fundamental theory, algorithms and codes — by fostering collaboration among different groups, by organizing scientific meetings and training schools, by coordinating applications for large computational facilities throughout Europe, and by engaging with the industry and policymakers. Another ambitious grass-roots initiative is the European Materials Modelling Council (EMMC) that aims to bring together the different materials modelling activities in Europe and to increase European industrial competitiveness by enhancing the use of modelling in this sector[9].

Similar bottom-up initiatives have also been developed on a more local scale. The Thomas Young Centre (TYC), for instance, was founded as an alliance of different London-based groups working on materials' theory and simulations[10]. One of the co-directors of the TYC, Angelos Michaelides from University College London, explains in an Interview on page 371 the current challenges in modelling materials and the objectives of the centre. On page 381, Nicola Marzari from the École Polytechnique Fédérale de Lausanne, discusses the broad range of topics debated during the Frontiers of Materials Modelling Symposium, held in February 2016 in London to celebrate the TYC's tenth anniversary, as well as current limitations on the accuracy of simulations, the complexity of *ab initio* models implemented and computational power.

The financial support, the improvement of codes, algorithms and methods, and the access to large computational facilities made possible by both governmental actions and the cooperation of the research community, are helping to tackle many of these challenges[2]. Yet, as explained by Michaelides, involvement from experimental groups is crucial for the field to move forward. At present, limited access to experimental raw data constitutes a serious hurdle for many modelling groups. Actions to overcome this issue have been taken. In 2014, for example, Springer Nature launched *Scientific Data*, an open-access, peer-reviewed journal that publishes descriptions of accessible good-quality raw experimental datasets, helping to make them more discoverable, interpretable and reusable[11]. In addition, full availability of experimental data and computer codes upon request is increasingly a requirement for many publications, including *Nature* journals[12]. Still, much work must be done in this regard to encourage experimentalists to share valuable scientific data in order to push forward materials modelling. ❐

References

1. https://www.whitehouse.gov/mgi
2. *Nature Mater.* **12,** 173 (2013).
3. https://materialsproject.org/
4. http://ec.europa.eu/research/industrial_technologies/modelling-materials_en.html
5. http://ec.europa.eu/programmes/horizon2020/en/area/key-enabling-technologies
6. http://ec.europa.eu/programmes/horizon2020/en
7. Goldbeck, G. *Industry Interactions of the Electronic Structure Research Community in Europe* (Goldbeck Consulting, 2014).
8. http://psi-k.net/
9. https://emmc.info/
10. http://www.thomasyoungcentre.org/
11. http://www.nature.com/sdata/
12. http://www.nature.com/authors/policies/availability.html