MAR17-2016-020363

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

DFT, Its Impact on Condensed Matter and on "Materials-Genome" Research[1]

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About 40 years ago, two seminal works demonstrated the power of density-functional theory (DFT) for real materials. These studies by Moruzzi, Janak, and Williams on metals [1] and Yin and Cohen on semiconductors [2] visualized the spatial distribution of electrons, predicted the equation of state of solids, crystal stability, pressure-induced phase transitions, and more. They also stressed the importance of identifying trends by looking at many systems (e.g. the whole transition-metal series). Since then, the field has seen numerous applications of DFT to solids, liquids, defects, surfaces, and interfaces providing important descriptions and explanations as well as predictions of experimentally not yet identified systems. –\\ About 10 years ago, G. Ceder and his group [Ref. 3 and references therein] started with high-throughput screening calculations in the spirit of what in 2011 became the "Materials Genome Initiative". The idea of high-throughput screening is old (a key example is the ammonia catalyst found by A. Mittasch at BASF more than 100 years ago), but it is now increasingly becoming clear that big data of materials does not only provide direct information but that the data is structured. This enables interpolation, (modest) extrapolation, and new routes towards understanding [Ref. 5 and references therein]. –\\ The amount of data created by "computational materials science" is significant. For instance, the NoMaD Repository [4] (which includes also data from other repositories, e.g. AFLOWLIB and OQMD) now holds more than 18 million total-energy calculations. In fact, the amount of data of computational materials science is steadily increasing, and about hundred million CPU core hours are nowadays used every day, worldwide, for DFT calculations for materials. –\\ The talk will summarize this enormous impact of DFT on materials science, and it will address the next steps, e.g. the issue how to exploit big data of materials for doing forefront research, how to find (hidden) structure in the data in order to advance materials science, identify new scientific phenomena, and to provide support towards industrial applications.

1. V.L. Moruzzi, J.F. Janak, and A.R. Williams, Calculated Electronic Properties of Metals (Pergamon, New York, 1978).

2. M.T. Yin and M.L. Cohen, PRB **26**, 5668 (1982).

3. A. Jain, K.A. Persson, and G. Ceder, APL Mater. **4**, 053102 (2016).

4. https://NOMAD-Repository.eu

5. L.M. Ghiringhelli *et al.*, PRL **114**, 105503 (2015); and New Journal of Physics, to be published.

[1]The NOMAD Laboratory Center of Excellence, European Unions Horizon 2020 research and innovation program, grant agreement no. 676580