Molecular Modelling 2.0

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Abstract

The ability to perform predictive quantum mechanical calculations using Density Functional Theory (DFT) [1] has transformed our understanding of materials at the atomic scale. The availability of many easy-to-use computer codes that implement DFT, such as CASTEP [2], has allowed widespread application of the method across numerous scientific disciplines and applications both in academia and industry. The success of methodology is such that the output of scientific publications which include the results of DFT calculations is now measured in kilo-papers per year! [3]

In this talk, I will present a personal view of how I believe the field of Molecular Modelling needs to evolve if it is to provide even greater real-world benefit in the future. Given the significant amounts of public funding that have been allocated to this research field in numerous countries, I am concerned that the academic research community will have to generate - and demonstrate - a significantly higher level of return on this investment than is currently achieved, in order to justify the same degree of support in the future.

References

[1] Hohenberg, P. & Kohn W. Inhomogeneous electron gas. Physical Review. 136, B864 (1964); Kohn, W. & Sham, L.J. Self-consistent equations including exchange and correlation effects. Physical Review. 140 A1133 (1965).

[2] https://www.castep.org/

[3] A search on Web-of-Science for `[(DFT)or "density functional theory") (Topic) AND (material*) or (solid*) (Topic)]` covering the most recent 5-year period (2020-2024) yields 52,557 hits, and a search for the whole 40-year period before this (1979-2019) yields 49,400 hits. [Search performed 10 January 2025]