Turkish Journal of Physics

Volume 39 | Number 3 Article 12

1-1-2015

Two common terminological mistakes in scientific papersTwo common terminological mistakes in scientific papers

ŞAKİR ERKOÇ

TÜBİTAK

Turkish Journal of Physics

http://journals.tubitak.gov.tr/physics/

Letter to the Editor

Turk J Phys
(2015) 39: 314 – 315

doi:10.3906/fiz-1506-27

Two common terminological mistakes in scientific papers

Şakir ERKOÇ*
Department of Physics, Middle East Technical University, Ankara, Turkey

Received: 26.06.2015 • **Accepted/Published Online:** 19.08.2015 • **Printed:** 30.11.2015

There are some common terminological mistakes in some scientific papers published in some peer-reviewed journals. It is difficult to understand why such mistakes exist in peer-reviewed journals. It seems that the review of scientific papers is not done as well as it should be.

One common mistake is made in papers containing the interpretation of electronic structure calculations of molecules, clusters, and/or nanoparticle-like finite systems. For instance, in some cluster papers the authors mention the "Fermi level" of the system they investigate. It is a mistake to mention the Fermi level of a finite system such as an atom, molecule, or cluster. Fermi level, Fermi energy, and Fermi surface are defined and meaningful for periodic systems, not for finite systems. The reason for this comes from the definition, where these expressions are defined in reciprocal space. Reciprocal space is defined for periodic structures [1]. For finite systems instead of "Fermi level" one should use the expression "highest occupied level". For instance, for molecules the highest occupied level has a special name, HOMO, highest occupied molecular orbital. Similarly, the expressions "band structure" and "band gap" exist in cluster papers. These are also terminological mistakes. These mistakes probably come from using package programs in the calculations. Some package programs are originally developed for periodic systems, and they calculate all possible properties, including Fermi energy, etc. Using such a program one can also calculate some finite system properties by taking a larger periodic working cell. People usually take the data generated by the package program and put them into their papers without considering the physical meaning of the generated numbers. There is the exception of Fermi energy for finite systems, which is used in nuclear physics. Fermi energy is well defined for nuclei [2], which is also a finite system. However, the Fermi energy expression used in nuclear physics is based on the Fermi gas model, which was originally developed for the electronic properties of metals [1].

Another common mistake is made in molecular dynamics simulation type papers. In some molecular dynamics simulation papers authors mention "molecular dynamics simulations are performed at T=0 Kelvin". Such an expression is also a mistake. The molecular dynamics method does not work at zero temperature. The method that works at zero temperature is called the "static method", not molecular dynamics. These two methods are quite different from each other [3]. This mistake probably comes from running the molecular dynamics program at very low temperature, less than 1 Kelvin. A small temperature value is a "small temperature", not zero temperature; a "very small value" is not equivalent to a "zero value".

The authors, the reviewers, and even more importantly the editors should pay more attention to the terminologies used in scientific papers.

*Correspondence: erkoc@metu.edu.tr

Acknowledgment

The author would like to thank the anonymous referee for calling the attention of the author to the nuclear physics problem.

References

[1] Ashcroft, N. W.; Mermin, N. D. *Solid State Physics;* Holt-Saunders International Editions: New York, NY, USA, 1976.

[2] Friedlander, G.; Kennedy, J. W.; Miller, J. M. *Nuclear and Radiochemistry;* 2nd Ed., Wiley: New York, NY, USA, 1964.

[3] Rapaport, D. C. *The Art of Molecular Dynamics Simulation;* Cambridge University Press: Cambridge, UK, 1995.