The History and the Development of some CoGEF comments

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April 24, 2026

This short text concerns the 2026 Comment (number 129 in my paper's list):

Wolfgang Quapp and Josep Maria Bofill: Commentary on "A systematic workflow for mechanophore design" in MRS Communications of the publisher Springer Nature. Today, it is a singular event that a serious comment was accepted. We thank the journal, the editor, and the reviewers. To understand our Comment, please look in it directly. We argue that the CoGEF method often results in false jumps uncontrollable over the PES.

There is, of course, a long prehistory: In 1998 we came down at what the later so called Newton trajectories (NT):
[1] Wolfgang Quapp, Michael Hirsch, Olaf Imig, Dietmar Heidrich: Searching for Saddle Points of Potential Energy Surfaces by Following a Reduced Gradient,
J. Comput. Chem. **19**, (1998), 1087-1100 (my most cited paper).
[2] Wolfgang Quapp, Michael Hirsch, Dietmar Heidrich: Bifurcation of Reaction Pathways: the Set of Valley Ridge Inflection Points of a Simple Three-dimensional Potential Energy Surface, Theor. Chem. Acc. **100**, (1998), 285-299.

The fundamental idea is that a curve is searched for where the gradient at every point of a potential points into the same direction. This method replaces and improves upon the 'distinguished coordinate method' [3-5].
[3] Klaus Müller and L.D. Brown: Location of Saddle Points and Minimum Energy Paths by a Constrained Simplex Optimisation Procedure, Theor. Chim. Acta, **53**, (1979), 75-93.
[4] I. H. Williams and G. M. Maggiora: Use and Abuse of the Distinguished-Coordinate Method For Transition-State Structure Seraching, J. Mol. Struct. (Theochem), **89**, (1982), 365-378.
[5] D.Heidrich: An Introduction to the Nomenclature and Usage of the Reaction Path Concept, in: The Reaction Path in Chemistry, (Ed.: D.Heidrich), Kluwer Academic Press, Dordrecht, 1995, p.1-10.

The papers [1,2] had, so to say, rediscovered the wheel. Mathematicians were already familiar with the theory [6]. For this reason, we later renamed the reduced gradient following (RGF) into Newton trajectories.
[6] Immo Diener: Globale Aspekte des kontinuierlichen Newtonverfahrens, Habilitation, Göttingen, 1991;
and H.Th. Jongen, P. Jonker and F. Twilt: Nonlinear Optimization in Finite Dimensions, Kluwer Academic Publ., Dordrecht Boston London, 2000.

NTs can be used to find all stationary points on a potential surface because they connect such points [1,2,7], as well as bifurcation points of valleys, compare also
[7] R. Crehuet, J. M. Bofill and J. M. Anglada: A new Look at the Reduced-gradient-following Path, Theor. Chem. Acc., **107**, (2002), 130-139.

There are many applications of the method to different problems. Still later, the method was applied to mechanochemistry [8], a very natural application.
[8] W.Quapp and J. M. Bofill: A contribution to a theory of mechanochemical pathways by means of Newton trajectories, Theoret. Chem. Acc., **135**, (2016), 113.

Currently (2025), the old, flawed distinguished coordinate method is being revived through the use of the so-called CoGEF method, see the cited comment above, (as bad as similar methods). In the comment we cite a long list of papers with an similar error. Thus, a not overly difficult mathematical method that follows the NTs, is being replaced by an even simpler, but often false going method. This method makes often incorrectly uncontrollable jumps across the potential surface. The incriminated points are turning points well known for Newton trajectories.

And some chemists reject my hints. xxx xxx xxx xxx xxx xxx xxx xxx xxx xxx xxx xxx xxx

It was the reason for the comment above, but we made additionally a famous test of the performance of different journals to handle a comment against a clear error in accepted papers. Here we report the answer of five further editors which rejected our quasi equal comments to the CoGEF method.

1-2) Two comments, publisher Wiley

Comment on "Mechanochemical Diels–Alder Reactions: Conceptual Density Functional Theory and Information-Theoretic Analyses by
S. G. Patra, A. Poddar, R. Jha, S. S. Kadam, C. Paul, P. K. Chattaraj, *ChemPhysChem* **2025**, *26*, e202500019224103.
and
Comment on "Mechanoresponsive Metal- Organic Cage-Crosslinked Polymer Hydrogels" by R. Küng, A. Germann, M. Krüsmann, L. P. Niggemann, J. Meisner, M. Karg, R. Göstl, B. M. Schmidt, *Chem. Eur. J.* **2023**, *29*, e202300079.

The two journals are under the same publisher, and the two editors contacted vice versa and constated a self-plagitarianism of our comments. It was enouph to reject the comments, in both journals.

Our answer was not answered back:

Dear Dr. Partha Pratim Pal (Deputy Editors of ChemPhysChem)
Dear Dr. Kieran Schlegel-O'Brien (Editor of Chemistry - A European Journal)
You avoid a discussion of a faulty method in your journals. You reject the comments by a more 'advocatic' argument than by the search for scientific truth.

In contrast, since the error emerges on two different potential energy surfaces of two different chemical systems, this is a strong hint that the commented CoGEF method often works wrong, indeet. The given 'rupture forces' are false values. Should they stay uncommented?

A solution could be that we combine the two comments to one comment.

3) Publisher Elsevier

Comment on ''Evaluating the predictive character of the method of constrained geometries simulate external force with density functional theory" by
C. R. Wick, E. Topraksal, D. M. Smith, A.-S. Smith, Forces in Mechanics 9 (2022) 100143.

The rejection's reason is the most stupid I ever obtained:
Ange Therese Akono, Ph.D.
Editor-in-Chief (Forces in Mechanics)
Editor and Reviewer comments:
We regret to tell you we were not able to find the required number of reviewers to evaluate your manuscript; we don't want to delay the process for you any longer.

4) Publisher ACS

Comment on "Competitive activation experiments reveal significantly different mechanochemical reactivity of furanmaleimide and anthracenemaleimide mechanophores"
by
Luo, S.M., Barber, R.W., Overholts, A.C., Robb, M.J.: ACS Polym. Au 3, 202208 (2023)

Answer by:
Prof. Sébastien Perrier
Deputy Editor (ACS Polymers Au)
Thank you for submitting to ACS Polymers Au. I would like to apologize for the delay in handling your manuscript, as we were discussing this situation extensively.

At this time, we are going to proceed with rejecting your manuscript, but want to offer two options available to you:

1) Contact the Corresponding Author of 10.1021/acspolymersau.2c00047 with your comments. If the original authors agree, then a correction to their published manuscript might be appropriate.

2) Completely replicate the original study, with your suggested methodology. If you can prove errors in the original study, then an updated article or correction might be appropriate.

Please let me know if you have any questions.

WQ: Yes, my question is: how You think about scientific correctness?

5) Publisher Elsevier again

Comment on "Molecular dynamics model of mechanophore sensors for biological force measurement" by S. Mittal, R.E. Wang, R. Ros, A.E. Ondrus, A. Singharoy, Heliyon **11**, e41178 (2025)

The journal demands from the beginning money, also for this comment. The submission system does not accept a comment without the accepted bill for payment. It is to remark that the submission process itself was very tricky: Many non-understandable demands are coming, but at least we could the comment submit.

However, after a long time emerged a question:

Dear Editor of Heliyon,
We would like to inquire about the status of our comment, manuscript number HELIYON-D-25-12784. We cannot understand why a one-page text, pointing out an obvious error in the cited Figure, requires 100 days for processing time.

Answer:
Hello!
Thank you for contacting Elsevier Researcher Support.
To help us jump right into the solution, please ensure you have provided as much information as possible.
While you wait, you can take a look at our Journal Article Publishing Support Center where you can review FAQs and 'how to' videos.
To help ensure a fast response, please do not change the subject line of this email when replying. For any future correspondence, remember to quote your unique reference number provided in the subject line.
Regards,
Elsevier Researcher Support

Das ist doch sehr erfrischend! How funny is the submission of a comment.

At 26.3.2026 the rejection, without any useful explanation:
Dear DR. Quapp,
Thank you for submitting your manuscript to Heliyon. After careful evaluation, I regret to inform you that your manuscript is not suitable for publication, and I must therefore reject it. We encourage you to review the Guide for Authors of Heliyon and Elsevier's policies (https://www.elsevier.com/authors/policies-and-guidelines) for guidance on publication criteria.
We appreciate you submitting your manuscript to Heliyon and thank you for giving us the opportunity to consider your work.
Kind regards,
Heliyon
Comments: ??? non ???
Have questions or need assistance?

Answer: Yes , but I do not expect any replay. I guess that Elsevier's policies do not accept comments, at all?

Facit

One of six journals reacts correctly about an error in a paper which has goen though the review processes. It is a dark result – does it be connected with these general times where presidents more often lie than speak the truth?

Some answers of scientists which are faced with the comment above

I wrote: Dear Authors of a commented paper, XXX.

This comment was rejected by the journal YYY with nonscientific reasons.

May be You could read the comment, try to understand it, and possibly make a correction to Your paper? (And mainly, avoid the error in the future!)

With regards

Wolfgang Quapp

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Von Pratim Chattaraj <pratim.chattaraj@gmail.com>

Datum 10.12.2025 07:13

Dear Dr. Quapp,

Thank you for your comments on our paper. We are aware of the Newton trajectory method. As a matter of fact we do teach this to our students and we will implement it in our future studies. We have seen that very recent articles use the CoGEF method: We mention some of them for your perusal :

1 I. M. Klein, C. C. Husic, D. P. Kovács, N. J. Choquette and M. J. Robb, J. Am. Chem. Soc., 2020, 142, 16364–16381.

2 T. Bettens, M. Alonso, P. Geerlings and F. De Proft, Phys. Chem. Chem. Phys., 2019, 21, 7378–7388.

3 A. Das and A. Datta, J. Am. Chem. Soc., 2023, 145, 13484–13490.

4 C. R. Wick, E. Topraksal, D. M. Smith and A.-S. Smith, Forces Mech., 2022, 9, 100143.

5 A. Bhusal, K. Adhikari and Q. Sun, RSC Mechanochemistry, 2024, 1, 413–421.

Hence, we have also used the same methodology for our study.

Thanks for providing us with your valuable feedback on our article.

Sincerely,

Prof. Pratim Kumar Chattaraj

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Von Bernd M. Schmidt <Bernd.Schmidt@hhu.de>

Datum 9.12.2025 14:41

Dear Dr. Quapp,

Thank you for your email and your interest in our work. I did not have enough time to thoroughly read your paper and the cited literature, but I will do so once this year calms down. I am a bit confused, since our work relies mostly on force-modified potential energy surface (FMPES), in addition to COGEF, which was mainly done as a comparison. Maybe also our wording in the original publication in CEJ 2024 was not careful enough in this regard. I talked to Jan Meisner this morning, who carried out the work, and he would like to talk to you if both of your schedules allow for it.

All the best for the upcoming holiday season.

Bernd Schmidt

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Two of five directly concerned authors answered, no one has thought on a correction of former papers.