



## Reply to comment on 'The Computational 2D Materials Database: high-throughput modeling and discovery of atomically thin crystals'

**Haastrup, Sten; Strange, Mikkel; Pandey, Mohnish; Deilmann, Thorsten; Schmidt, Per Simmendefeldt; Hinsche, Nicki Frank; Gjerding, Morten Niklas; Torelli, Daniele; Larsen, Peter Mahler; Riis-Jensen, Anders Christian**

*Total number of authors:*  
15

*Published in:*  
2D materials

*Link to article, DOI:*  
[10.1088/2053-1583/ab2f00](https://doi.org/10.1088/2053-1583/ab2f00)

*Publication date:*  
2019

*Document Version*  
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

### *Citation (APA):*

Haastrup, S., Strange, M., Pandey, M., Deilmann, T., Schmidt, P. S., Hinsche, N. F., Gjerding, M. N., Torelli, D., Larsen, P. M., Riis-Jensen, A. C., Gath, J., Jacobsen, K. W., Mortensen, J. J., Olsen, T., & Thygesen, K. S. (2019). Reply to comment on 'The Computational 2D Materials Database: high-throughput modeling and discovery of atomically thin crystals'. *2D materials*, 6(4), [048002]. <https://doi.org/10.1088/2053-1583/ab2f00>

---

### General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

COMMENTS AND REPLIES • **OPEN ACCESS**

## Reply to comment on ‘The Computational 2D Materials Database: high-throughput modeling and discovery of atomically thin crystals’

Recent citations

- [Proposal for Reconfigurable Magnetic Tunnel Diode and Transistor](#)  
Ersoy aolu *et al*

To cite this article: Sten Hastrup *et al* 2019 *2D Mater.* **6** 048002

View the [article online](#) for updates and enhancements.

**Going Greener Together....**

Search and buy our Green Production materials at [www.goodfellow.com](http://www.goodfellow.com)

**Goodfellow**  
GREEN PRODUCTION

Bio-degradable      Non-toxic

Bio-based      Derived from renewable sources

The advertisement features a background of green grass and a stylized brown factory with smoke. It includes icons for a recycling symbol, a radiation symbol, a leaf, and a globe. The text promotes 'Green Production materials' and lists four key attributes: Bio-degradable, Non-toxic, Bio-based, and Derived from renewable sources.

## OPEN ACCESS

RECEIVED  
16 April 2019REVISED  
12 June 2019ACCEPTED FOR PUBLICATION  
3 July 2019PUBLISHED  
24 July 2019

Original content from  
this work may be used  
under the terms of the  
[Creative Commons  
Attribution 3.0 licence](#).

Any further distribution  
of this work must  
maintain attribution  
to the author(s) and the  
title of the work, journal  
citation and DOI.



## COMMENTS AND REPLIES

## Reply to comment on 'The Computational 2D Materials Database: high-throughput modeling and discovery of atomically thin crystals'

Sten Haastrup<sup>1</sup>, Mikkel Strange<sup>1</sup>, Mohnish Pandey<sup>1</sup>, Thorsten Deilmann<sup>1</sup>, Per S Schmidt<sup>1</sup>, Nicki F Hinsche<sup>1</sup>, Morten N Gjerding<sup>1</sup>, Daniele Torelli<sup>1</sup>, Peter M Larsen<sup>1</sup>, Anders C Riis-Jensen<sup>1</sup>, Jakob Gath<sup>1</sup>, Karsten W Jacobsen<sup>1</sup>, Jens Jørgen Mortensen<sup>1</sup>, Thomas Olsen<sup>1</sup> and Kristian S Thygesen<sup>1,2</sup>

<sup>1</sup> CAMD, Department of Physics, Technical University of Denmark

<sup>2</sup> Center for Nanostructured Graphene (CNG), Technical University of Denmark

E-mail: [thygesen@fysik.dtu.dk](mailto:thygesen@fysik.dtu.dk)

**Keywords:** 2D materials, high-throughput, database, density functional theory

**Abstract**

In his comment Maździarz 2019 (2D Mater. 6 048001) raises doubts concerning the reliability of our test for dynamical (in particular elastic) stability of monolayer materials, which neglects the shear components of the stiffness tensor and only considers the sign of the planar stiffness coefficients. We agree that our analysis has not been complete, but find that it suffices in practice except for very few cases (less than 1% of the materials). Nevertheless, for completeness we are currently calculating the shear components of the elastic tensor for all the materials in the C2DB.

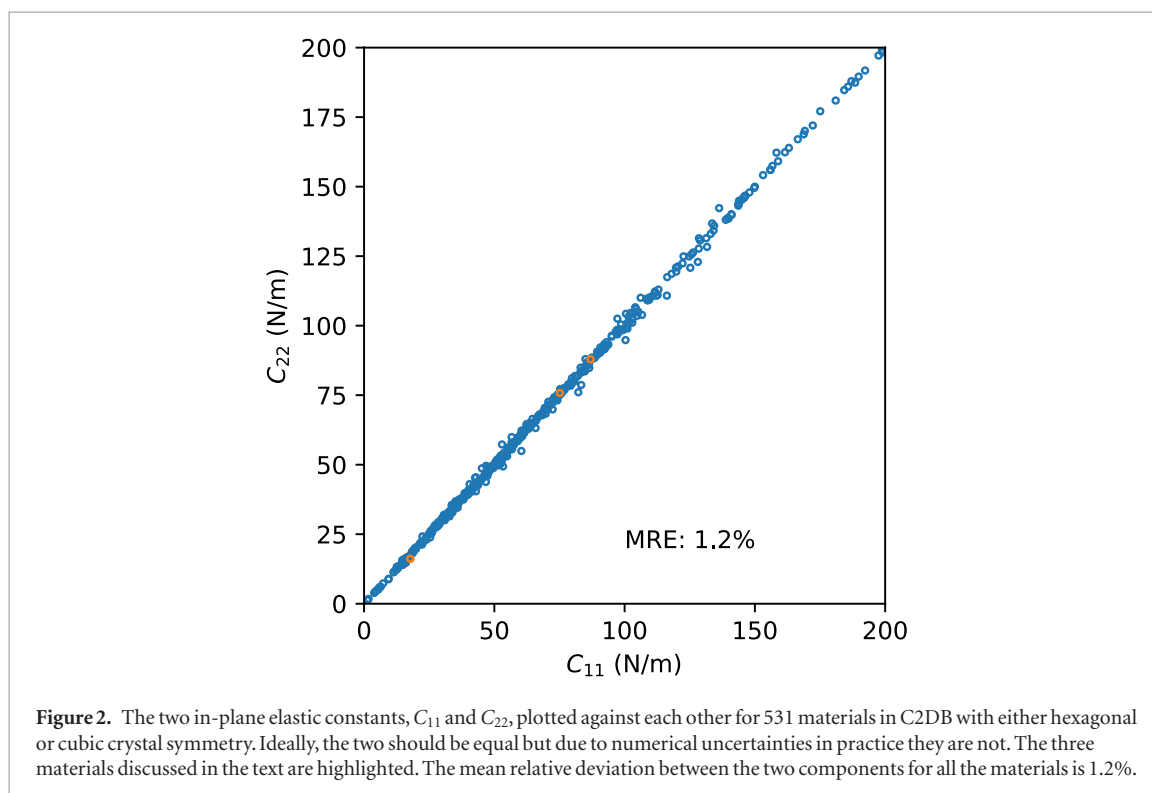
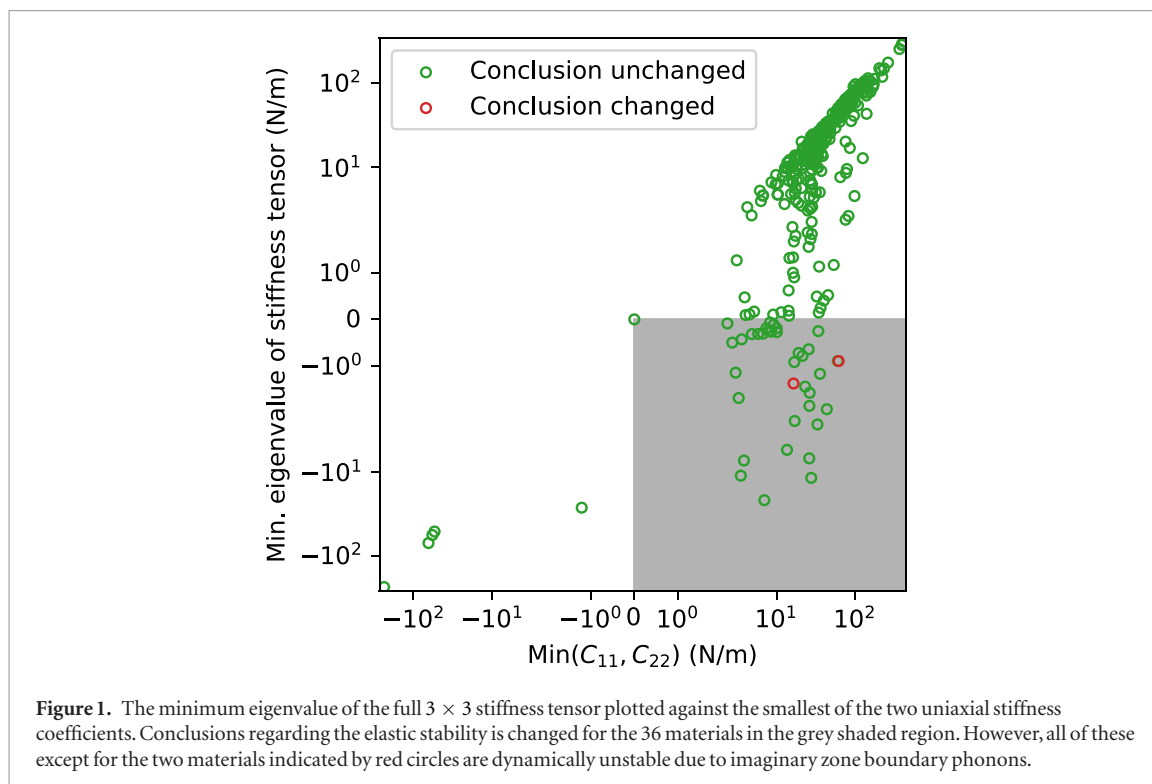
In our original paper [2], we described our strategy for testing whether a given hypothesized 2D material would be dynamically stable, i.e. whether it would spontaneously distort if all constraints imposed on the calculation (symmetries and unit cell size) were relaxed. In other words, the test for dynamical stability should assess whether the configuration of the given material represents a minimum or a saddle point of the potential energy surface. Regarding the atomic positions within the unit cell, we calculate the phonons at the corners of the Brillouin zone boundary (specifically the  $\Gamma$ -point phonons of the  $2 \times 2$  repeated cell). The material is classified as dynamically unstable if at least one phonon with imaginary frequency is found. Concerning the shape of the unit cell, we calculate the components of the stiffness tensor corresponding to uniaxial deformations along the  $x$ , and  $y$ -axis, namely the  $C_{11}$ ,  $C_{22}$ , and  $C_{12}$  components in the Voigt notation. A material is classified as dynamically unstable if either  $C_{11}$  or  $C_{22}$  is negative.

As pointed out in the comment, the correct test for dynamical stability would involve, in addition to the phonon analysis, a diagonalization of the full stiffness tensor to check for negative eigenvalues. By considering only the sign of  $C_{11}$  or  $C_{22}$  there is a risk that a material is incorrectly classified as dynamically stable when in reality it would undergo a shear deformation.

We have calculated the full  $3 \times 3$  stiffness tensor,  $C$ , for 378 materials in the C2DB. We picked this set of

materials because we already had calculated the shear deformations in connection with the calculation of their piezoelectric tensors. They cover representatives from all five types of 2D Bravais lattices. In figure 1 we show the minimum eigenvalue of  $C$  plotted against  $\min\{C_{11}, C_{22}\}$ . There are 36 materials in the grey shaded area where our original assessment of dynamical stability based on the  $C_{11}$  and  $C_{22}$  components is wrong. Most of these are materials in the  $\text{GeS}_2$  structure prototype. However, 34 of these have at least one imaginary zone boundary phonon and would therefore be classified as dynamically unstable in any case. Therefore, the stronger criterion based on the full stiffness tensor only leads to a different conclusion for two materials, namely  $\text{GeSe}_2$  in the  $\text{GeS}_2$  prototype and  $\text{I}_2\text{Sb}_2$  in the  $\text{CuI}$  prototype, which are now classified as dynamically unstable.

Maździarz highlights three specific materials from C2DB, namely  $\text{Au}_2\text{O}_2\text{-GaS}$ ,  $\text{Ta}_2\text{Se}_2\text{-GaS}$ , and  $\text{Re}_2\text{O}_2\text{-FeSe}$ , and criticises that (1) despite the hexagonal and cubic symmetries of the lattices  $C_{11}$  and  $C_{22}$  are not equal for these materials, and (2) the elastic stability of the crystals is not reflected by the signs of  $C_{11}$  and  $C_{22}$ . Regarding (1), we acknowledge that  $C_{11}$  and  $C_{22}$  should be equal in these cases, but according to our calculations they deviate by 1.1%, 0.8%, and 9%, respectively. The average deviation for the 531 materials in C2DB with hexagonal or cubic symmetry is 1.2%, see figure 2. This is obviously due to numerics



as we also write in our original paper (page 9): ‘for the isotropic materials  $\text{MoS}_2$ ,  $\text{WSe}_2$  and  $\text{WS}_2$ ,  $C_{11}$  and  $C_{22}$  should be identical, and we see a variation of up to 0.6%. This provides a test of how well converged the values are with respect to numerical settings.’ The deviation of 9% for  $\text{Re}_2\text{O}_2\text{-FeSe}$  is an outlier and we speculate that it arises due to the strong dynamical instability of this material (see below). We note that we could have decided to symmetrise the elastic tensors by hand such as to exactly reflect the symmetry of

the lattice. We have, however, refrained from such symmetrisation procedure because we believe it is relevant and more transparent to provide the raw rather than post-processed data. Similar considerations apply to many other quantities in C2DB. Regarding (2) we can essentially refer to the discussion in the first part of this paper. After calculating the full stiffness tensor for the three materials we obtain the same conclusions regarding the elastic stability of these materials as suggested in the Comment. However, as was the case for 99.5%

of the 378 test materials discussed above, irrespective of the stiffness tensor all three materials are correctly categorised as dynamically unstable in C2DB because they have zone boundary phonons with imaginary frequencies.

Despite the fact that only 0.5% out of the set of 378 materials are affected, we have decided to calculate the full stiffness tensor for all of the approximately 4000 materials currently in the C2DB. The full stiffness tensors for the 378 materials have already been made available in the C2DB, and data for the remaining materials will be available as soon as the calculations are done.

### Acknowledgments

The Center for Nanostructured Graphene is sponsored by the Danish National Research Foundation, Project DNRF103. This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 773122, LIMA).

### ORCID iDs

Sten Haastrup  <https://orcid.org/0000-0003-3696-0356>

Thorsten Deilmann  <https://orcid.org/0000-0003-4165-2446>

Nicki F Hinsche  <https://orcid.org/0000-0002-0176-6038>

Morten N Gjerding  <https://orcid.org/0000-0002-5256-660X>

Daniele Torelli  <https://orcid.org/0000-0002-4861-0268>

Thomas Olsen  <https://orcid.org/0000-0001-6256-9284>

Kristian S Thygesen  <https://orcid.org/0000-0001-5197-214X>

### References

- [1] Maździarz M 2019 *2D Mater.* **6** 048001
- [2] Haastrup S *et al* 2018 *2D Mater.* **5** 042002