



## Corrigendum: High throughput computational screening for 2D ferromagnetic materials: the critical role of anisotropy and local correlations (2D Mater. 6 045018)

Torelli, Daniele; Thygesen, Kristian S.; Olsen, Thomas

*Published in:*  
2D materials

*Link to article, DOI:*  
[10.1088/2053-1583/ab7bfb](https://doi.org/10.1088/2053-1583/ab7bfb)

*Publication date:*  
2020

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

[Link back to DTU Orbit](#)

*Citation (APA):*  
Torelli, D., Thygesen, K. S., & Olsen, T. (2020). Corrigendum: High throughput computational screening for 2D ferromagnetic materials: the critical role of anisotropy and local correlations (2D Mater. 6 045018). *2D materials*, 7, [049501]. <https://doi.org/10.1088/2053-1583/ab7bfb>

---

### 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.

**CORRIGENDUM**

**Corrigendum: High throughput computational screening for 2D ferromagnetic materials: the critical role of anisotropy and local correlations (2D Mater. [6 045018](#))**

To cite this article: Daniele Torelli *et al* 2020 *2D Mater.* **7** 049501

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



## CORRIGENDUM

## Corrigendum: High throughput computational screening for 2D ferromagnetic materials: the critical role of anisotropy and local correlations (2D Mater. 6 045018)

RECEIVED  
5 February 2020REVISED  
17 February 2020ACCEPTED FOR PUBLICATION  
3 March 2020PUBLISHED  
23 July 2020Daniele Torelli<sup>1</sup> , Kristian S Thygesen<sup>1,2</sup> and Thomas Olsen<sup>1</sup> <sup>1</sup> Computational Atomic-scale Materials Design (CAMD), Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark<sup>2</sup> Center for Nanostructured Graphene (CNG), Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark**Keywords:** 2D magnetism, high throughput calculations, first principles calculations

**Table 1.** List of 2D magnetic insulating materials with positive exchange coupling  $J$  and positive spinwave gap  $\Delta$ . Structure denotes the prototypical crystal structure and  $S$  is the spin carried by each magnetic atom. The critical temperature  $T_C$  is obtained from equation 5 of the original manuscript. The top part of the table contains dynamically and thermodynamically stable materials. The lower part of the table contains materials that are not expected to be stable in their pristine form but exhibit high critical temperatures.

Formula	Structure	$J$ [meV]	$\Delta$ [meV]	$S$ [ $\hbar$ ]	$T_C$ [K]
FeCl <sub>2</sub>	MoS <sub>2</sub>	15.2	0.056	2.0	208
CuCl <sub>3</sub>	BiI <sub>3</sub>	15.3	0.058	1.0	37
CrI <sub>3</sub>	BiI <sub>3</sub>	2.3	0.96	1.5	35
CoCl <sub>2</sub>	CdI <sub>2</sub>	2.0	0.058	1.5	31
CrBr <sub>3</sub>	BiI <sub>3</sub>	2.0	0.23	1.5	23
MnO <sub>2</sub>	CdI <sub>2</sub>	0.54	0.31	1.5	19
NiCl <sub>2</sub>	CdI <sub>2</sub>	7.2	0.001	1.0	14
CrCl <sub>3</sub>	BiI <sub>3</sub>	1.4	0.033	1.5	13
RuCl <sub>2</sub>	MoS <sub>2</sub>	18.7	2.3	2.0	606
RuBr <sub>2</sub>	MoS <sub>2</sub>	16.1	1.77	2.0	509

In the original manuscript a small error in the calculation of exchange coupling constants was introduced due to different versions of the code being

used for ferromagnetic and anti-ferromagnetic configurations. The error also propagated into the calculated spin-wave gaps and critical temperatures, which was summarized in Table 2 of the original manuscript. This only affected PBE calculations, but not the PBE+U calculations. In Table 1 we provide the corrected values. Except for MnO<sub>2</sub> all values are in close proximity to the ones reported in the original manuscript. For MnO<sub>2</sub> the corrected value for the critical temperature is 19 K, which is much lower than the value of 63 K reported previously.

## ORCID iDs

Daniele Torelli <https://orcid.org/0000-0001-6256-9284>Kristian S Thygesen <https://orcid.org/0000-0002-4861-0268>Thomas Olsen <https://orcid.org/0000-0001-5197-214X>