

## Supplementary Information

### Ferromagnetic clusters in the monoclinic modification of TaFeTe<sub>2</sub> layered van der Waals telluride

Anna V. Stepanova,<sup>a</sup> Andrey N. Azarevich,<sup>b</sup> Alexey V. Bogach,<sup>b</sup> Maria A. Kirsanova,<sup>c</sup>  
Tatyana M. Vasilchikova,<sup>d</sup> Olga S. Volkova,<sup>d</sup> Danil S. Plenkin,<sup>a</sup> Andrei V. Shevelkov,<sup>a</sup>  
Valeriy Yu. Verchenko<sup>\*a</sup>

<sup>a</sup>Department of Chemistry, Lomonosov Moscow State University, 119991 Moscow, Russia

<sup>b</sup>Prokhorov General Physics Institute of the Russian Academy of Sciences, 119991 Moscow, Russia

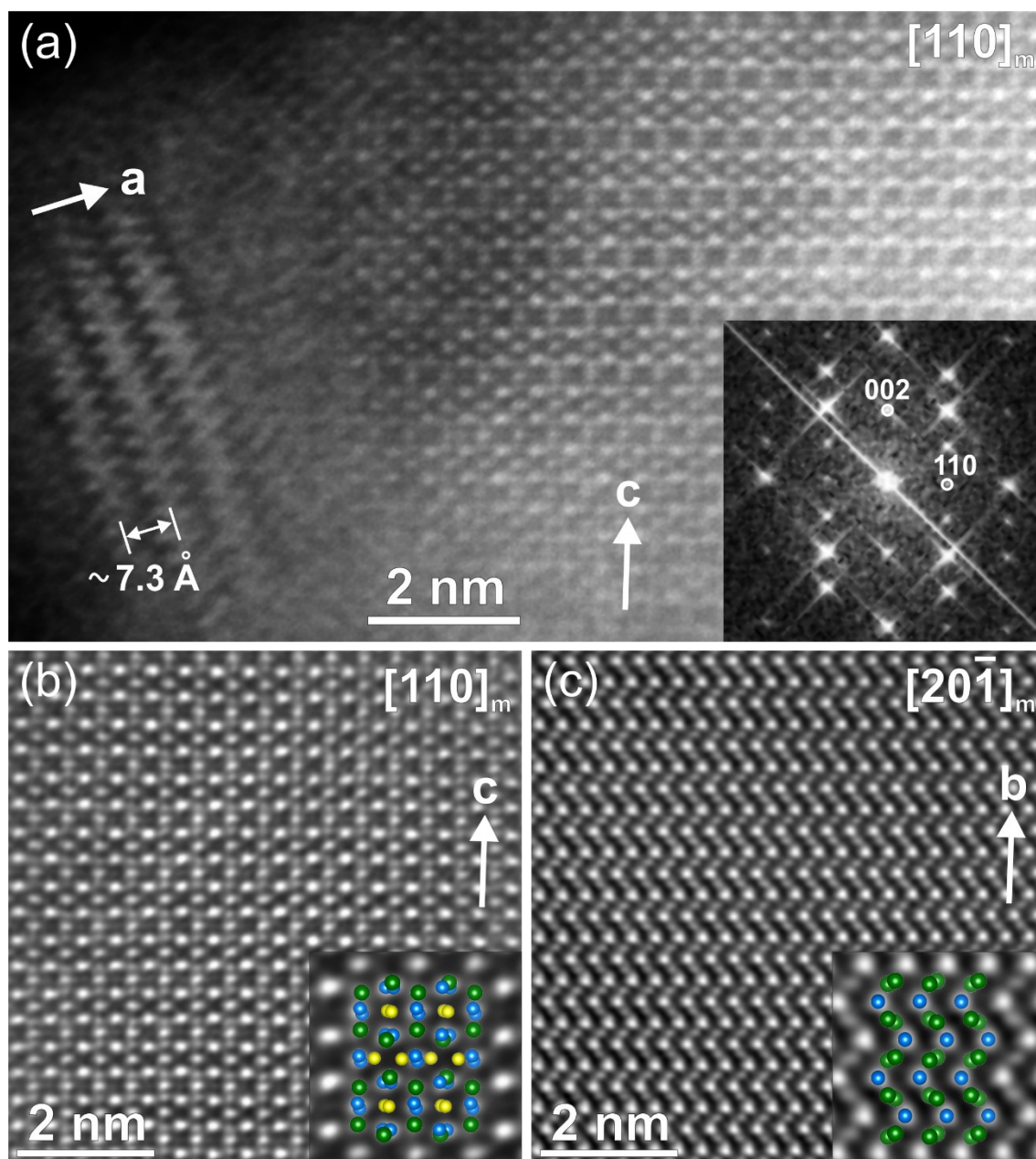
<sup>c</sup>Advanced Imaging Core Facility / Center for Energy Science and Technology, Skolkovo Institute  
of Science and Technology 121205 Moscow, Russia

<sup>d</sup>Department of Physics, Lomonosov Moscow State University, 119991 Moscow, Russia

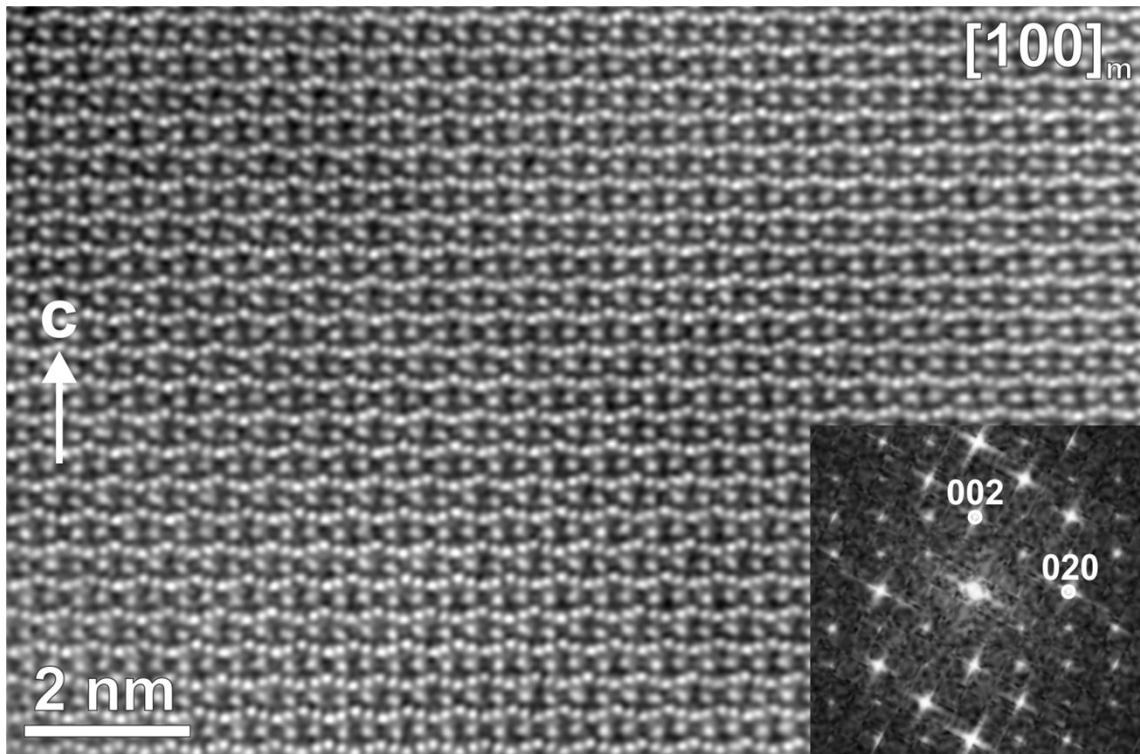
\*valeriy.verchenko@gmail.com

**Table S1.** Optimized structural parameters of monoclinic TaFeTe<sub>2</sub> [ $P2_1/c$ ,  $a = 7.272 \text{ \AA}$ ,  $b = 6.107 \text{ \AA}$ ,  $c = 8.185 \text{ \AA}$ ,  $\beta = 94.06^\circ$ ] within the ferromagnetic ground state.

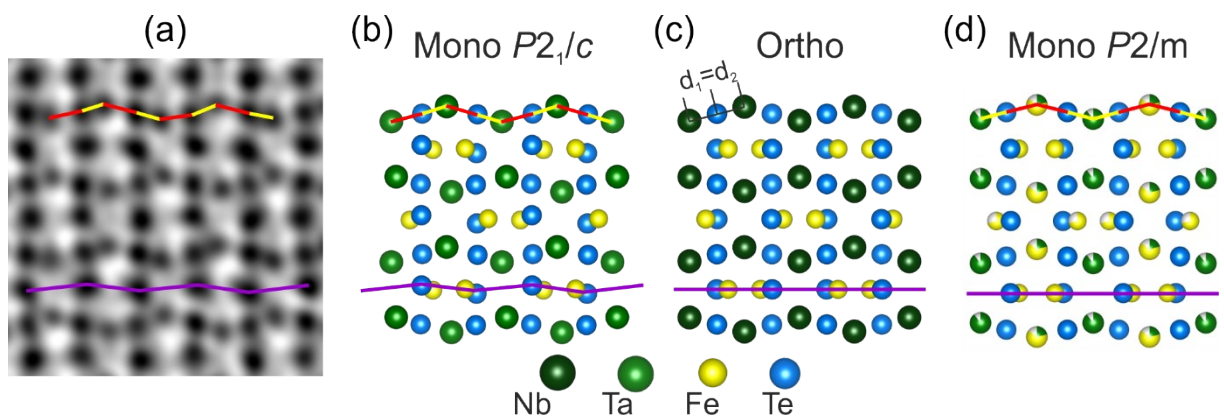
Site	Wyckoff	$x$	$y$	$z$	Magnetic moment ( $\mu_B$ )
Ta1	$4e$	0.0220	0.5306	0.1918	-0.23
Fe1	$4e$	0.1002	0.3510	0.4910	1.47
Te1	$4e$	0.3150	0.2437	0.2491	0
Te2	$4e$	0.2383	0.7548	-0.0331	0



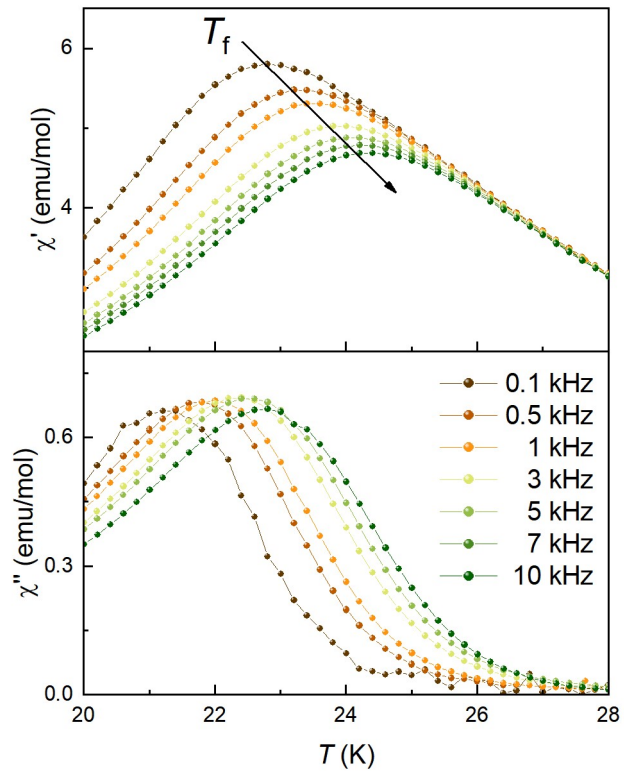
**Figure S1.** (a) HAADF-STEM image taken from the thin TaFeTe<sub>2</sub> crystal mainly oriented along the [110]<sub>m</sub> direction. The crystallographic planes in the left part of image are packed along the *a* axis. FFT in inset clearly shows 00*l*: *l* = 2*n* reflection condition. (b, c) [110]<sub>m</sub> and [201]<sub>m</sub> HAADF-STEM images with superimposed projections of the monoclinic crystal structure of TaFeTe<sub>2</sub>.



**Figure S2.**  $[100]_m$  HAADF-STEM image taken from the thin  $\text{TaFeTe}_2$  crystal illustrating the atomic arrangement characteristic for monoclinic structure. FFT in the inset evidences  $0k0$ :  $k = 2n$  and  $00l$ :  $l = 2n$  reflection conditions.



**Figure S3.** (a) ABF-STEM image of  $\text{TaFeTe}_2$  and projections of the (b) monoclinic  $P2_1/c$ , (c) orthorhombic and (d) monoclinic  $P2/m$   $\text{MFeTe}_2$  ( $M = \text{Nb}, \text{Ta}$ ) structures. Experimental ABF-STEM image clearly evidences zigzag arrangement of Te/Fe atomic columns (violet line) and alternation of long (red) and short (yellow) projected Ta-Te distances. Only the monoclinic  $P2_1/c$  model is consistent with this image.



**Figure S4.** Real and imaginary parts of ac magnetic susceptibility of the TaFeTe<sub>2</sub> non-oriented crystals at various frequencies in the vicinity of freezing temperature.