

SUPPORTING INFORMATION

Non-thermal Magnetic Deicing Using Two-Dimensional Chromium Telluride

Chinmayee Chowde Gowda¹, Alexey Kartsev^{2,3,4}, Nishant Tiwari⁵, Safronov A.A.³, Prafull Pandey⁶, Ajit K. Roy⁷, Pulickel M. Ajayan⁸, Douglas S. Galvão^{9*} and Chandra Sekhar Tiwary^{1,5}*

¹School of Nano Science and Technology, Indian Institute of Technology Kharagpur, West Bengal – 721302, India

²Computing Center of the Far Eastern Branch of the Russian Academy of Sciences, 680000 Khabarovsk, Russia

³MIREA-Russian Technological University, 119454 Moscow, Russia

⁴Peoples' Friendship University of Russia (RUDN University), 6 Miklukho-Maklaya St, Moscow 117198, Russia

⁵Department of Metallurgical and Materials Engineering, Indian Institute of Technology Kharagpur, West Bengal – 721302, India

⁶Materials Engineering, Indian Institute of Technology Gandhinagar, Gujarat – 382055, India

⁷Materials and Manufacturing Directorate, Air Force Research Laboratory, Wright Patterson AFB, Ohio, 45433-7718, USA

⁸Department of Materials Science and NanoEngineering, Rice University, 6100 S Main Street, Houston, TX 77005, USA

⁹Applied Physics Department and Computational Engineering and Sciences, State University of Campinas, Campinas, SP, 13083-970, Brazil

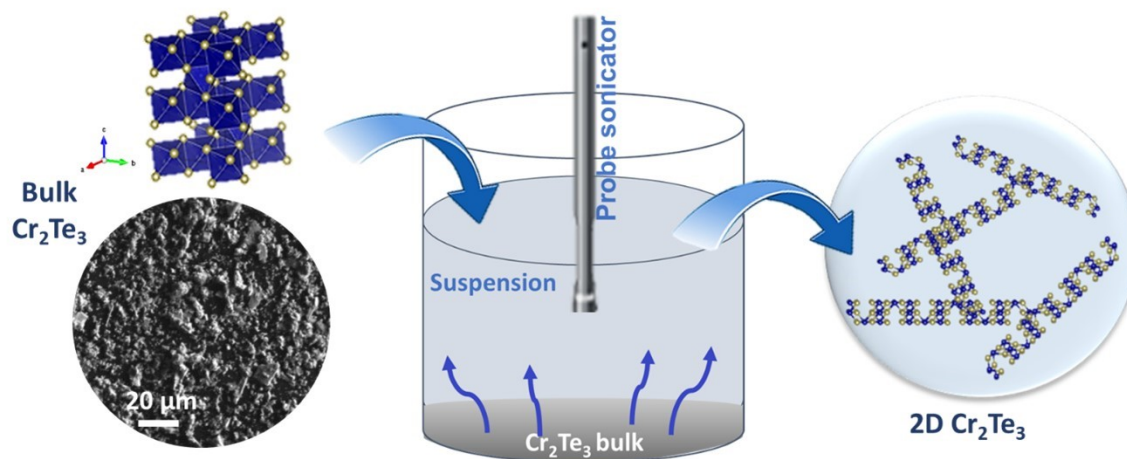


Figure S1: Schematic representation of the liquid phase exfoliation technique (inset down: SEM image of bulk Cr_2Te_3 crushed sample).

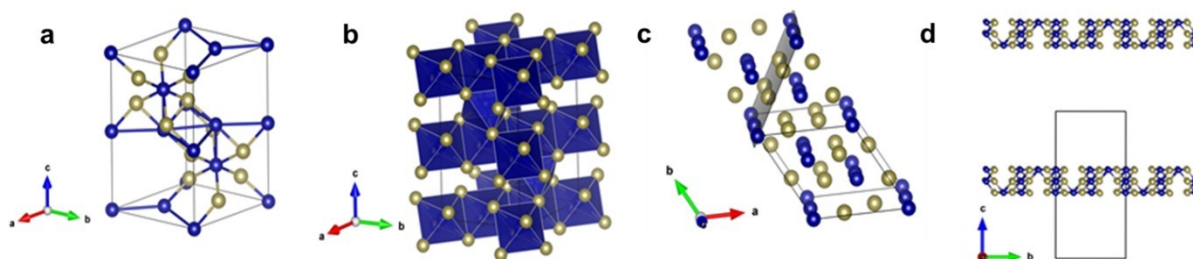


Figure S2: Volumetric view of the original structure, (a) Cr atoms are shown in blue, Te atoms in yellow, (b) volumetric view of the original structure in the polyhedron model, (c) plane $(11\bar{0})$ in the original structure and (d) initial 2D structure.

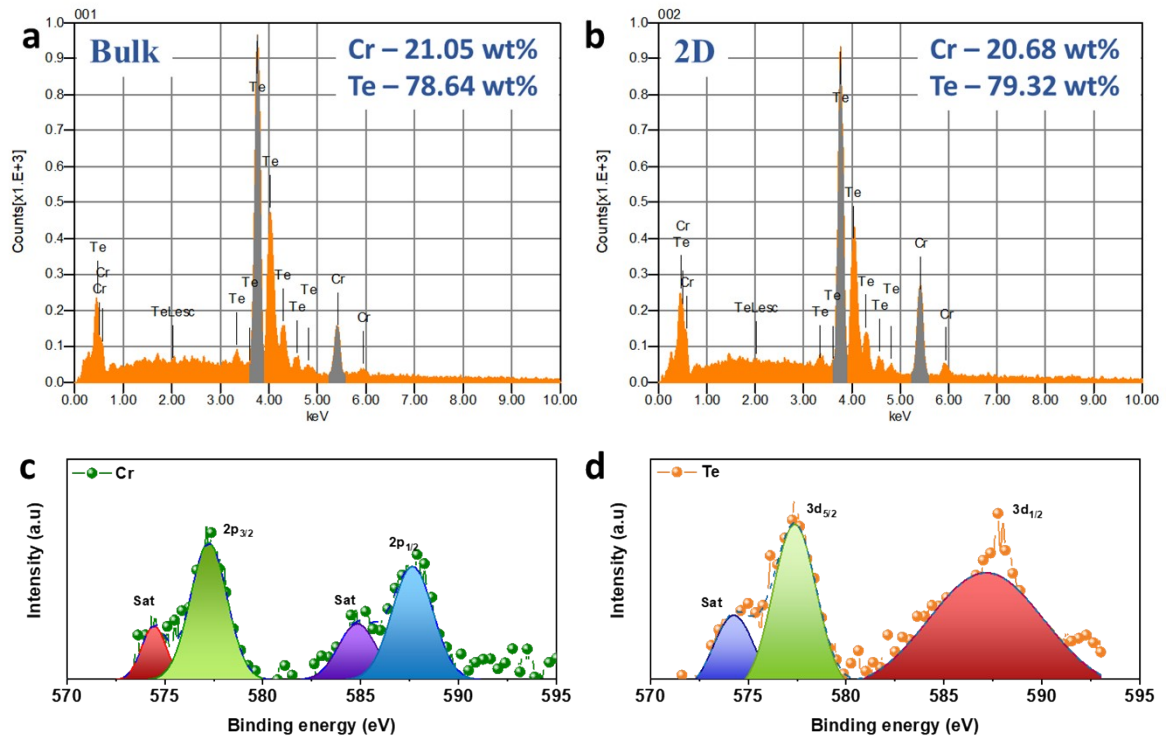


Figure S3: Elemental analysis of (a) bulk sample after homogenization, and (b) 2D Cr_2Te_3 , (c) XPS survey spectra of Cr_2Te_3 (c) Chromium and (d) Tellurium.

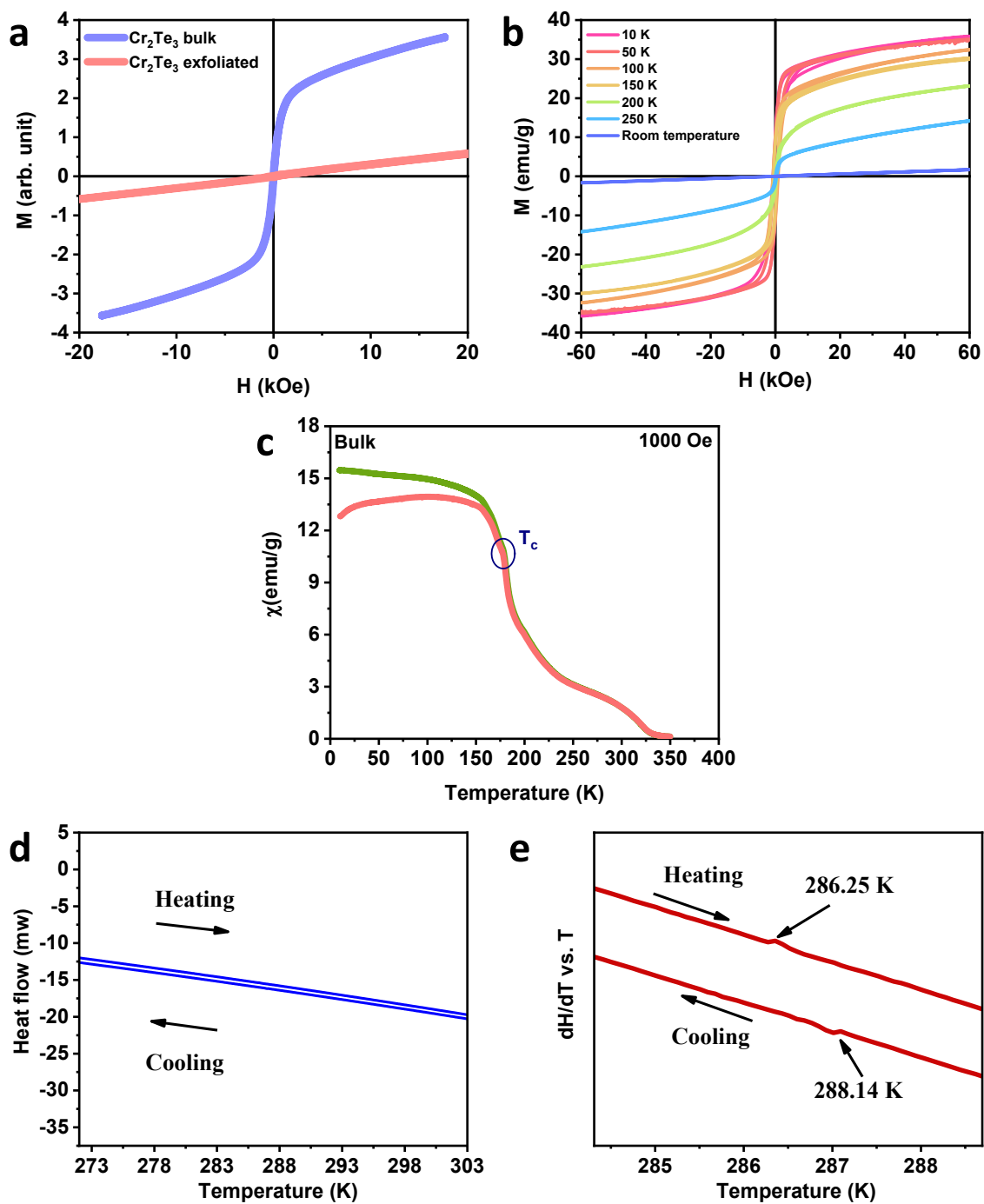


Figure S4: Magnetic behavioural studies (a) M - H loop of bulk and 2D Cr_2Te_3 at room temperature, (b) M - H loop at temperatures ranging from 10 K to 300 K (50 K intervals) and (c) FC-ZFC curves depicting T_c at 180 K for bulk Cr_2Te_3 (d) DSC data showing heating and cooling curves and (e) dH/dT vs. T curves.

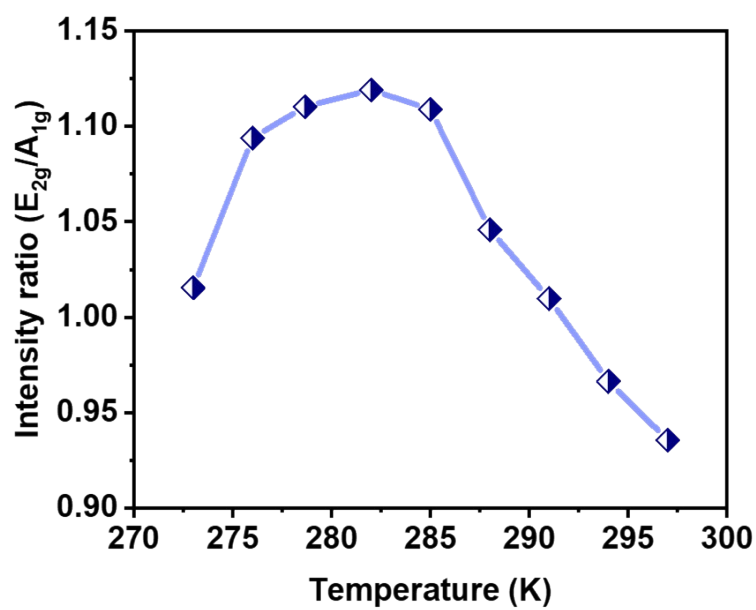


Figure S5: Intensity ratio shift of two major Raman bands during heating conditions (273 K to 297 K).

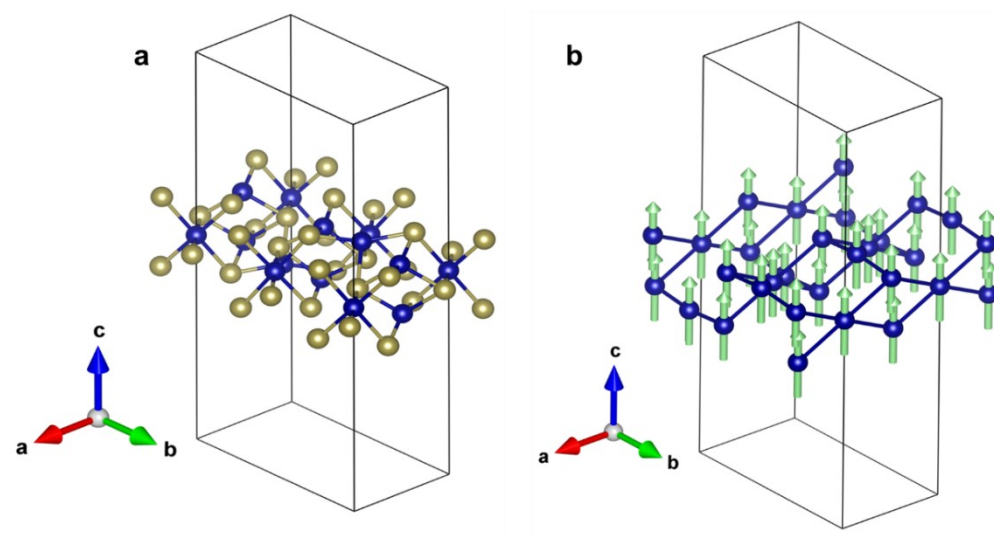


Figure S6: (a) Final view of the 2D structure Cr_2Te_3 and (b) magnetic sublattice Cr.

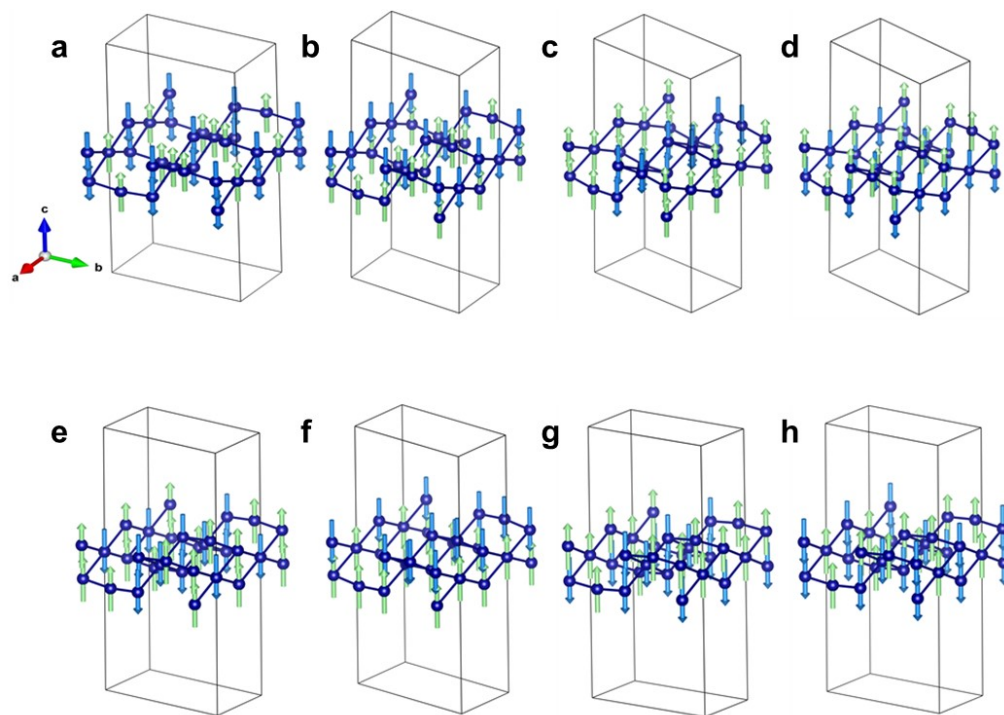


Figure S7: Magnetic sublattice Cr of the final system with possible orientations of the spin magnetic moment in the antiferromagnetic structure (a-h).

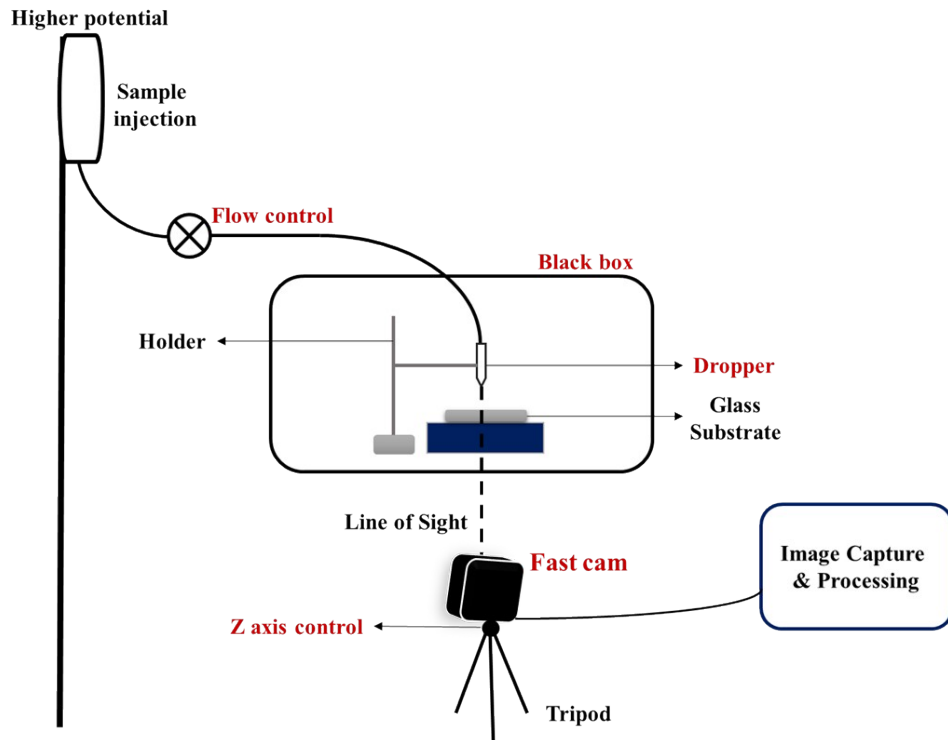


Figure S8: Schematic diagram of 2D Cr_2Te_3 drop on glass substrate for wettability study.

High speed camera specifications:

Model: Fastcam Mini UX 50 type 160 K – M – 4G

Frame rate: 2000 fps

Shutter speed: 1/ frame sec

Resolution: 1280 x 1024

Frame count: 2180 frame

Rec duration: 1.09 sec

Trigger mode: Start

Zoom ratio: 422 % (Variable)

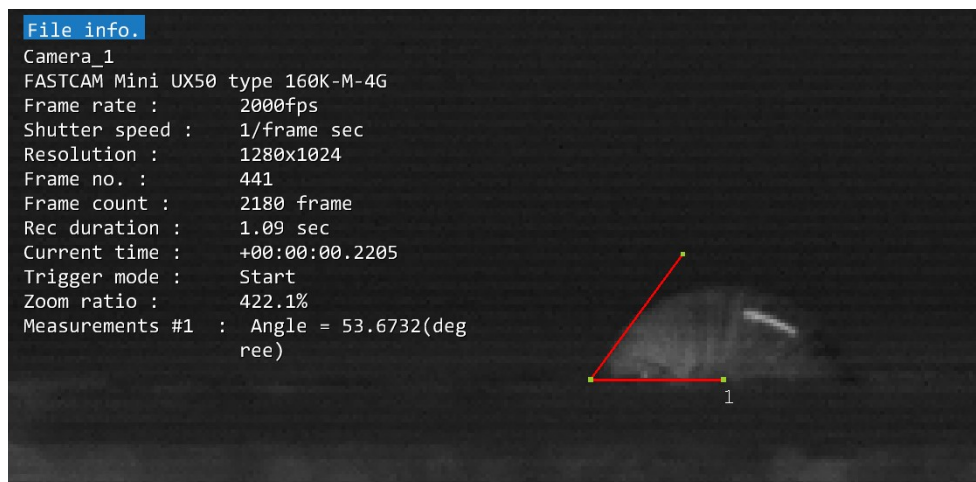


Figure S9: Single frame captured during measurement of water contact angle (Bulk Cr_2Te_3 in this case) from Photron photo viewer software (PFV4 ($\times 64$)).

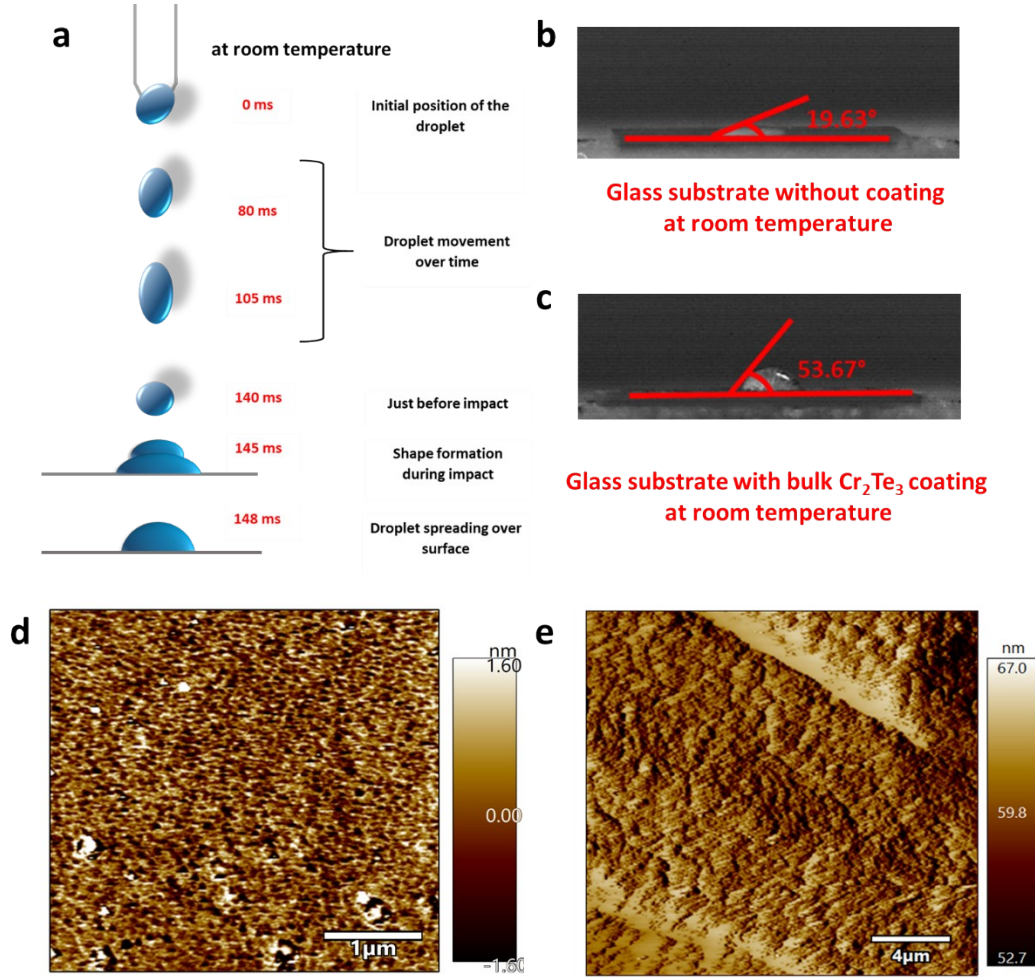


Figure S10: (a) Schematic representation of water drop falling on a surface, Contact angle measurement on (b) plane glass substrate and (c) bulk Cr_2Te_3 coating, Surface morphology obtained by AFM (d) 2D Cr_2Te_3 and (e) Bulk Cr_2Te_3 .

Surface Interaction studies:

We have considered two cases of ice attachment to chromium telluride (**Figure S11**). The formation energy E^{form} of the 1L- $\text{H}_2\text{O}/\text{Cr}_2\text{Te}_3$ structure was calculated as follows:

$$E^{\text{form}} = E^{\text{tot}}(1\text{L} - \text{H}_2\text{O}/\text{Cr}_2\text{Te}_3) - E^{\text{tot}}(1\text{L} - \text{H}_2\text{O}) - E^{\text{tot}}(1\text{L} - \text{Cr}_2\text{Te}_3) \quad (\text{S1})$$

where, $E^{\text{tot}}(1\text{L-H}_2\text{O/Cr}_2\text{Te}_3)$, $E^{\text{tot}}(1\text{L-H}_2\text{O})$ and $E^{\text{tot}}(1\text{L-Cr}_2\text{Te}_3)$ are the total energies of 1L- $\text{H}_2\text{O/Cr}_2\text{Te}_3$ structure, ice crystal monolayer and 1L- Cr_2Te_3 monolayer, respectively. The obtained vdW gap values between the Cr_2Te_3 and H_2O layers are 1.9 and 2.3 Å for the ferromagnetic and paramagnetic structure, respectively. The formation energies of different combinations are tabulated in **Table S1**.

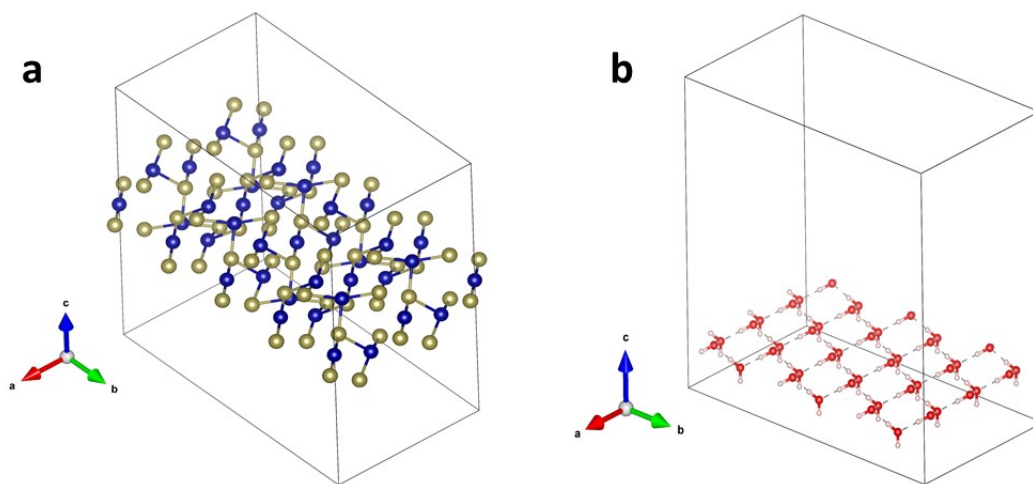


Figure S11: (a) 1L- Cr_2Te_3 2×2 supercell and (b) 1L- H_2O 3×3 supercell

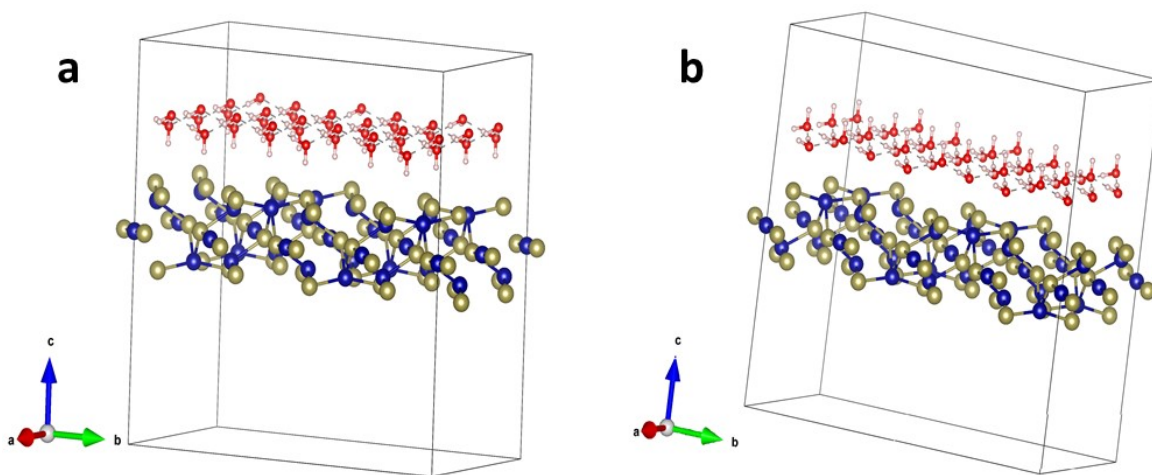


Figure S12: Two cases of ice attachment to chromium telluride. (a) Oxygen ions oriented towards the chromium telluride plane (O-oriented), (b) hydrogen ions oriented towards the chromium telluride plane (H-oriented).

Table S1. Structural parameters ($\alpha = 90^\circ$, $\beta = 90^\circ$) and calculated formation energy E^{form} for relaxed 1L- H_2O/Cr_2Te_3 heterostructures in four variants.

Structure	a, b (Å)	E^{form} (eV/ H_2O)
1L- H_2O/Cr_2Te_3 FM Cr_2Te_3 O-faced toward H_2O	a=12.72 b=23.49	0.242
1L- H_2O/Cr_2Te_3 FM Cr_2Te_3 H-faced toward H_2O	a=12.73 b=23.31	0.258
1L- H_2O/Cr_2Te_3 PM Cr_2Te_3 O-faced toward H_2O	a=12.57 b=23.29	0.390
1L- H_2O/Cr_2Te_3 PM Cr_2Te_3 H-faced toward H_2O	a=12.59 b=23.33	0.385

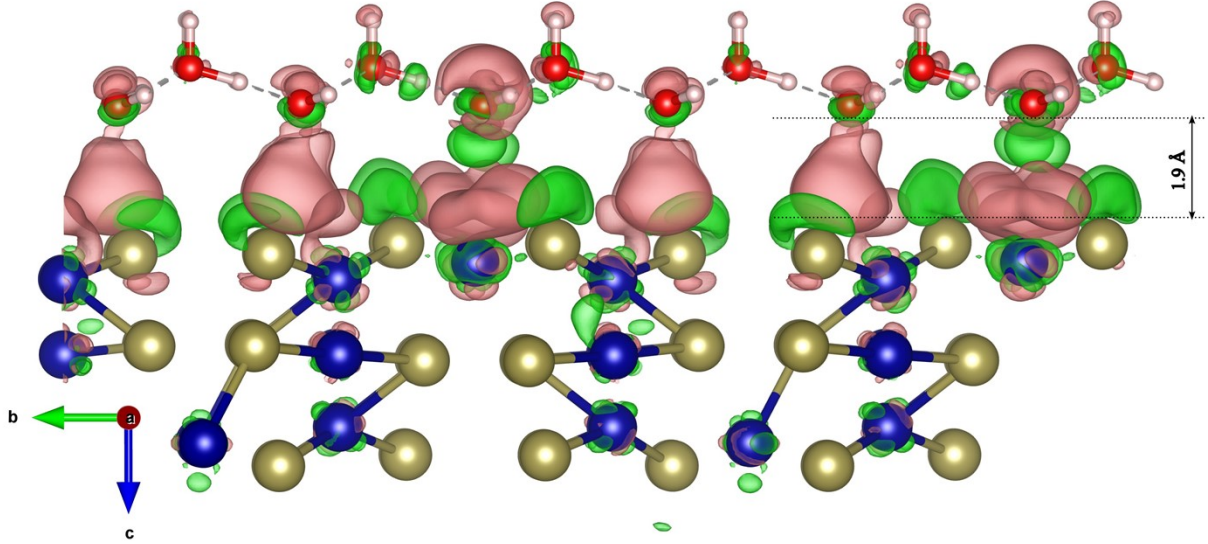


Figure S13: Charge transfer isosurface ($3 \cdot 10^{-4} e/\text{\AA}$) between ice and ferromagnetic Cr_2Te_3 monolayers. Red/green color correspond to the negative/positive charge difference. Dashed lines indicates the vdW gap between ice and substrate.

The charge transfer were computed using the following formalism:

$$\Delta\rho = \rho^{\text{Cr}_2\text{Te}_3/\text{H}_2\text{O}} - \rho^{\text{1Ltext-Cr}_2\text{Te}_3} - \rho^{\text{1Ltext-H}_2\text{O}} \quad (\text{S2})$$

where $\rho^{\text{Cr}_2\text{Te}_3/\text{H}_2\text{O}}$ is the charge density for the ice/ Cr_2Te_3 total monolayered structure, $\rho^{\text{1Ltext-Cr}_2\text{Te}_3}$ and $\rho^{\text{1Ltext-H}_2\text{O}}$ are charge density for the bare Cr_2Te_3 and bare H_2O monolayers, respectively. The charge transfer isosurface between ice and FM Cr_2Te_3 ML was $3 \times 10^{-4} e/\text{\AA}$.

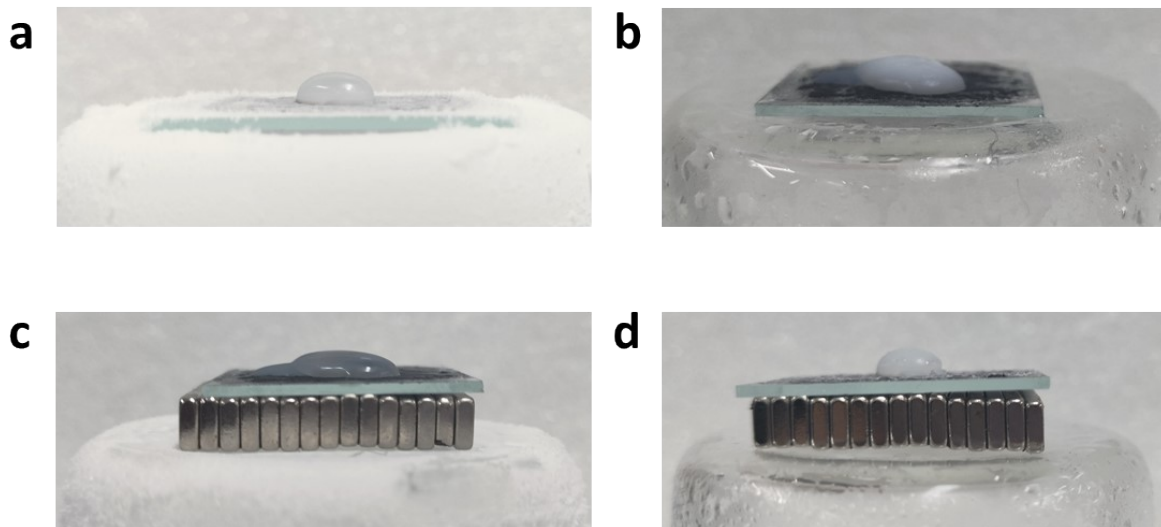


Figure S14: (a) Oil droplet on bare frozen surface (without magnetic field) at 0°C and (b) at Room temperature (> 25 °C), (c) Oil droplet on application of external magnetic field at 0°C and (d) at Room temperature (> 25 °C).