

Cross-plane thermal conductivity in MXenes

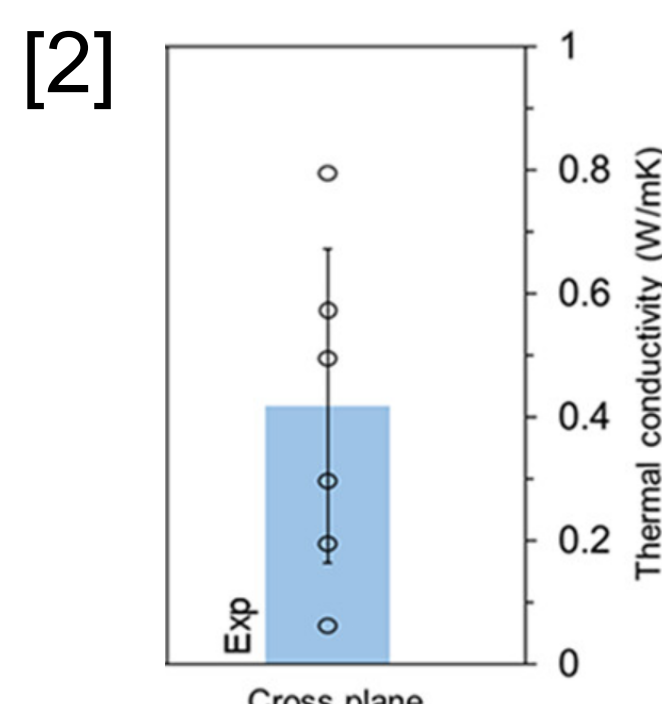
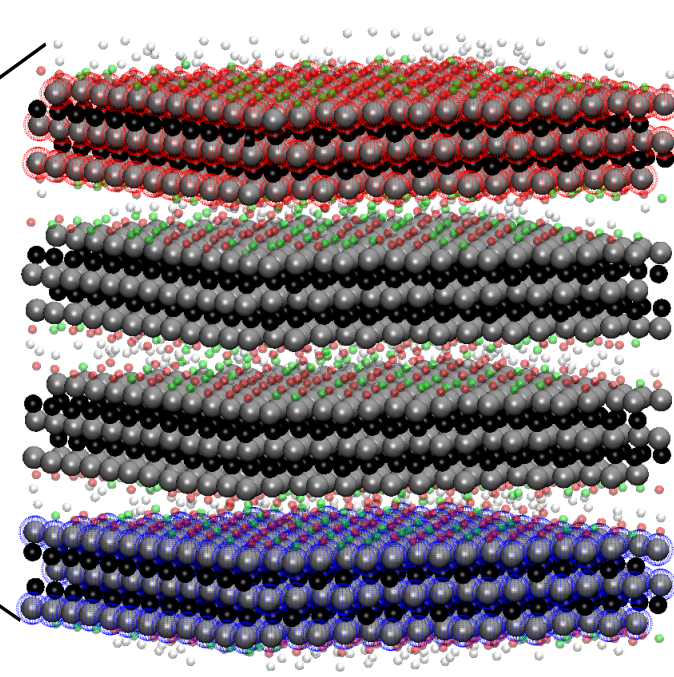
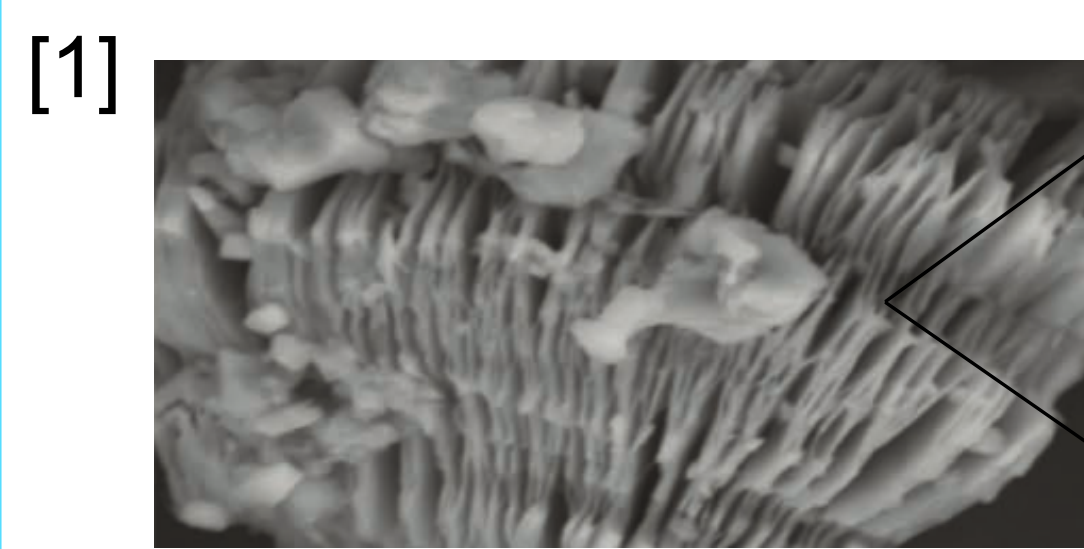
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1 - Introduction



Motivation

- > MXenes: 2D materials [1], with rich **surface chemistry**.
- > **Out-of plane thermal conductivity** measurements in MXenes spread over **one order of magnitude**. [2]
- > We show how MXenes **surface chemistry** affects their **thermal conductivity**.

2 - System and methods

Methodology

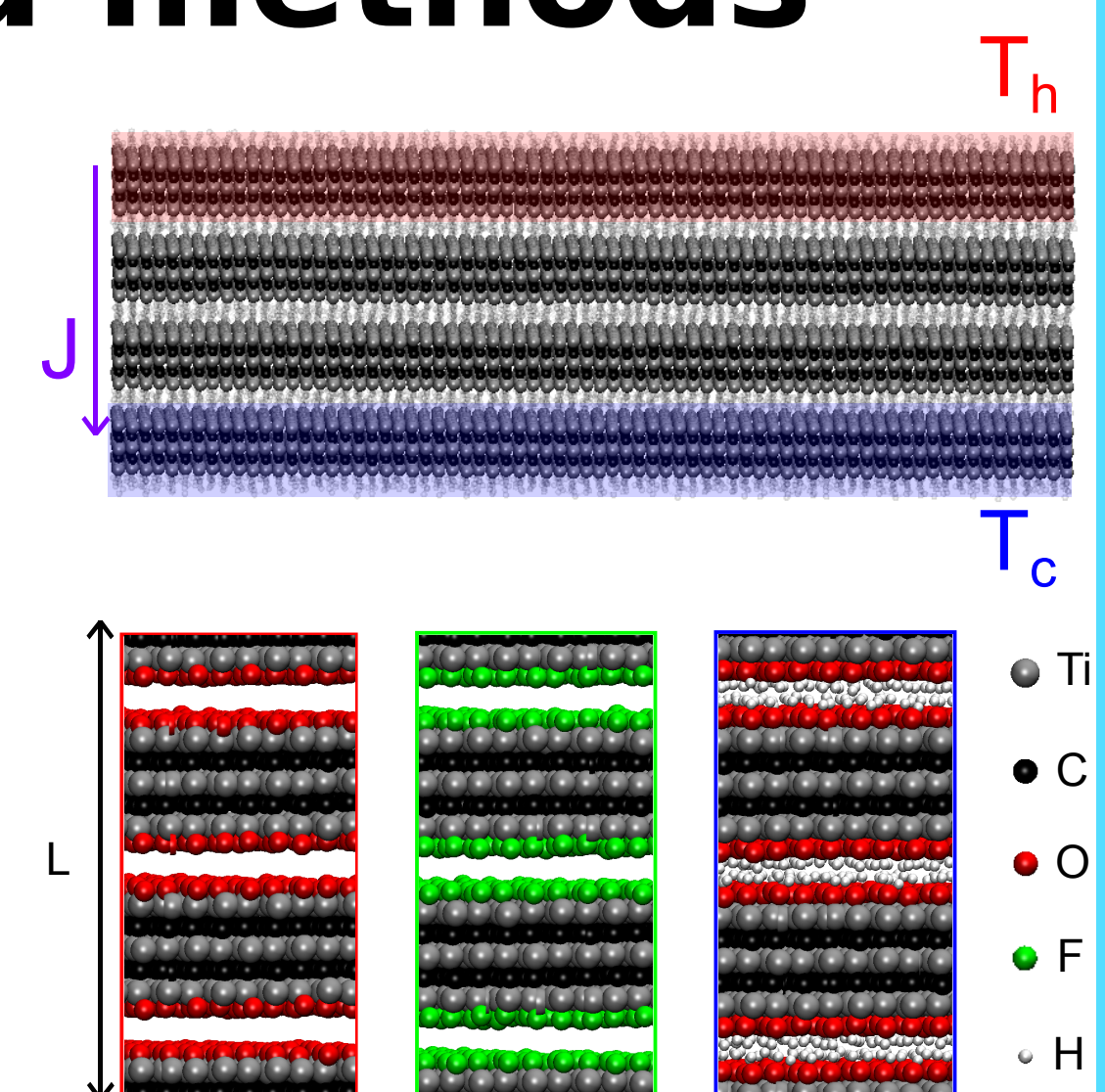
- > NEMD, LAMMPS.
- > Interface Force Field [3].

System

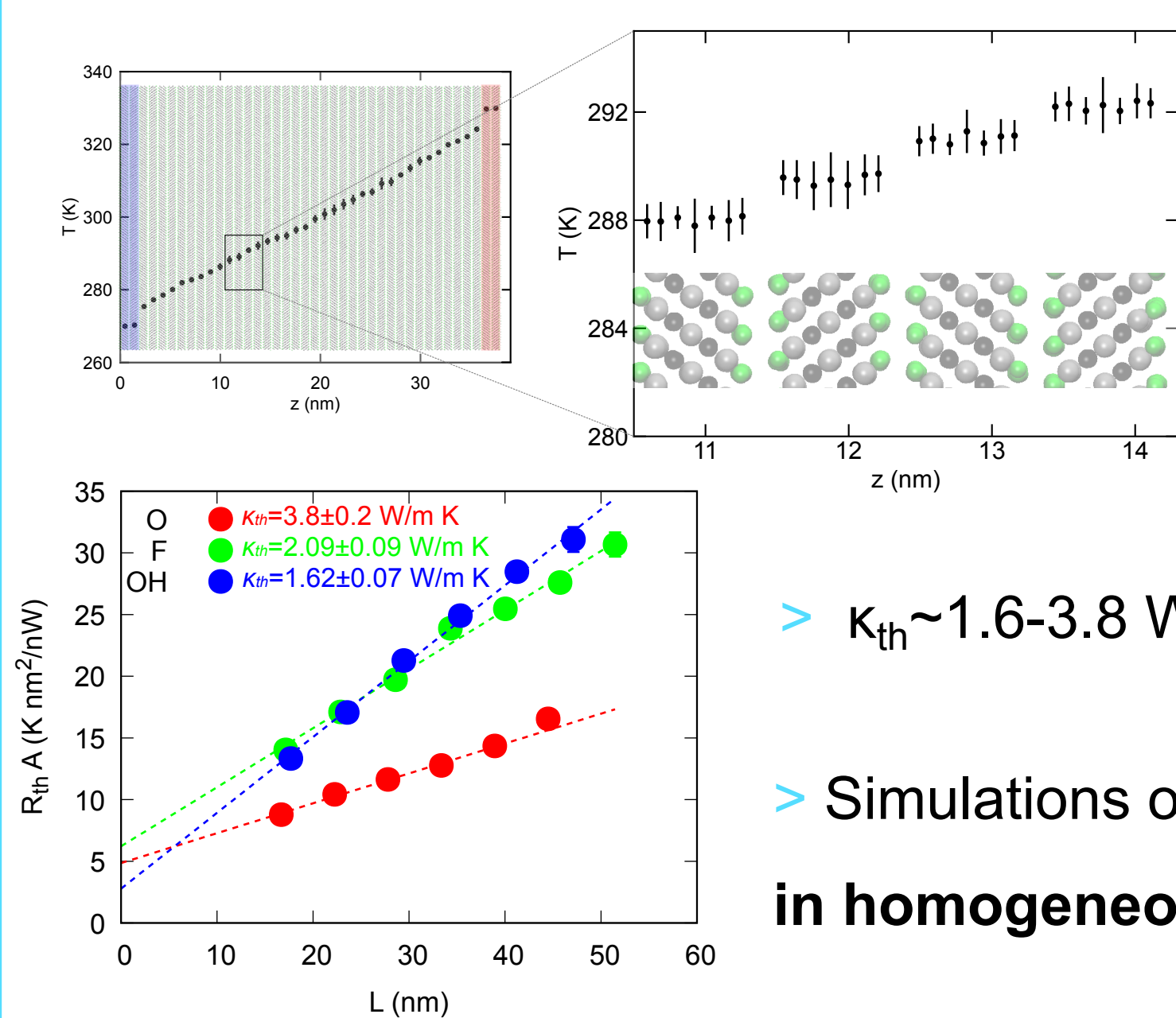
- > $Ti_3C_2T_x$ with **surface terminations**:
-F, -O, -OH

Protocol

- > **Heat flux** is imposed linking layers to different thermal baths: $\Delta T=60$ K.



3 - Homogeneous surfaces

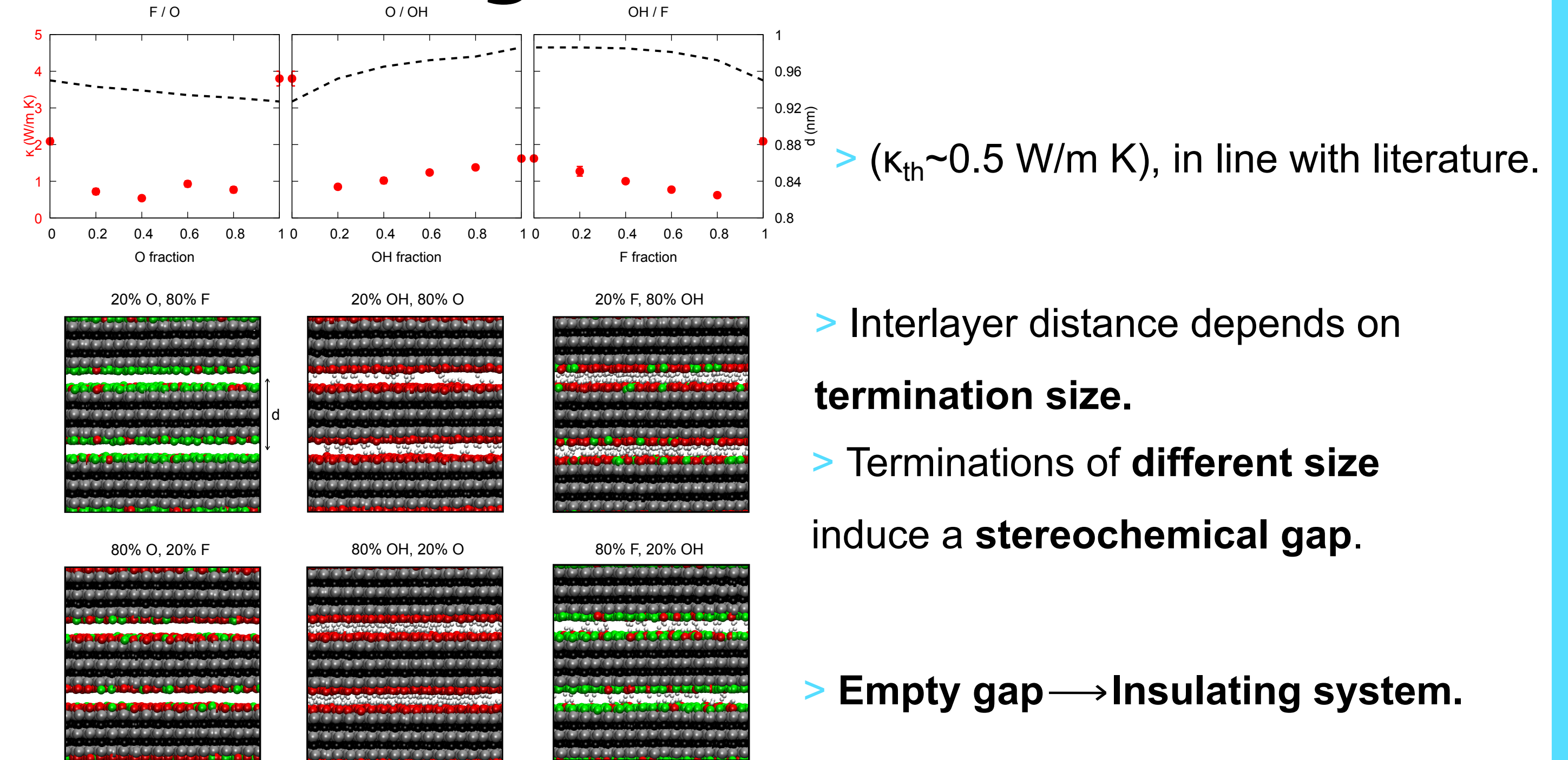


> Temperature jumps in the **interlayer space**.

> $\kappa_{th} \sim 1.6-3.8$ W/m K.

> Simulations overestimate conductivity in **homogeneous systems**.

4 - Heterogeneous surfaces

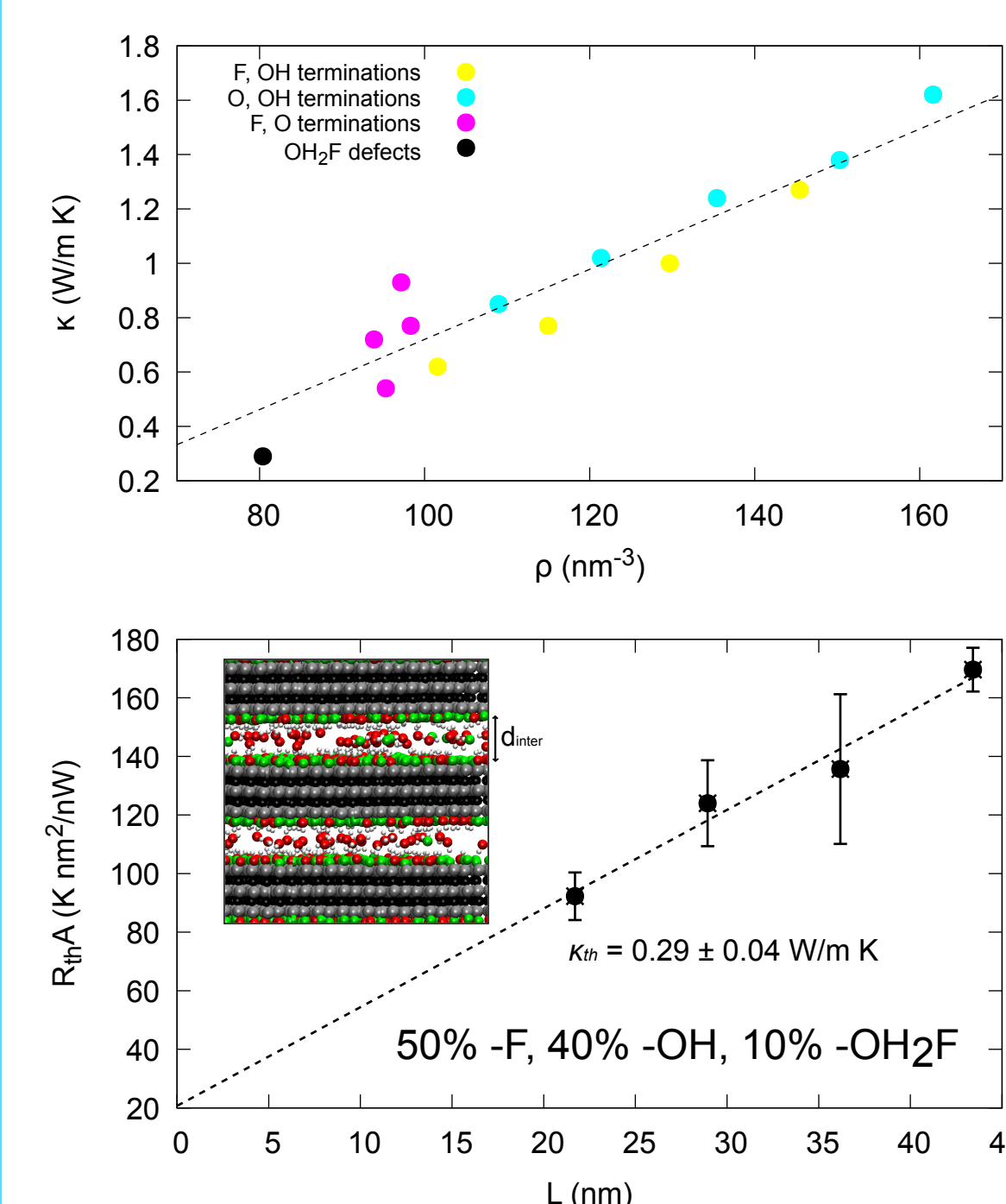


> Interlayer distance depends on **termination size**.

> Terminations of **different size** induce a **stereochemical gap**.

> **Empty gap** → **Insulating system**.

5 - The stereochemical gap



> Correlation between thermal conductivity and density in the interlayer space:

$$\rho = N_{atoms}/V_{inter}$$

> **Reducing density**, with **small proportions of large terminations**, thermal conductivity is more suppressed.

6 - Conclusions

- > Surface chemistry causes **one order of magnitude variability** on thermal conductivity.
- > Low thermal conductivity of MXenes is caused by a **stereochemical gap**, induced by different terminations.
- > Most insulating systems are achieved with a **low proportion of large terminations**.
- > Chemistry-driven route to engineer thermal transport.

References and acknowledgements

[1] M. Naguib *et al*, Advanced Materials, **23**, 4248-4253 (2011)

[2] T. Hassan, C. Park *et al*, ACS Nano, **19**, 40703-30732 (2025)

[3] I. Armstrong *et al*, <https://doi.org/10.26434/chemrxiv-2025-212s7>

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