

## The theoretical guidelines for optimized thermometry – An interplay between thermodynamics and kinetics for targeted design

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The overall goal of the EU-funded consortium NanoTBTEch is the development of new superior thermal imaging systems for applications in the biological sector. The organized webinar series gave a clear impression on what obstacles have to be overcome in order to achieve this challenging goal. The development of novel thermal imaging systems is a highly interdisciplinary field joining forces from materials science, chemistry, physics, biology and medicine. Within the webinar series, it became clear that the preparation and control of nanocrystalline materials with desired properties is of utmost importance. Artifacts in the temperature readout under real biological conditions are also a critical issue to be tackled carefully in practice. However, if properly controlled, luminescence nanothermometry proves to be a powerful tool. It was nicely demonstrated within this webinar how to use luminescence thermometry to elucidate new phase transitions within water, detect heat transport along lipid bilayers, or measure light-to-heat conversion at the micrometer scale in a remote manner. Promising luminescent nanomaterials for nanothermometry are especially lanthanide-doped fluorides, transition metal ion-doped oxides or semiconductor quantum dots.

Despite the impressively growing number of suggested materials for this purpose, a universal theoretical framework that covers the guidelines for an optimum thermometer performance and their applicability domains have been surprisingly lacking up to now. With such a framework, it would be possible to specifically design and target potential candidates for nanothermometry in a desired temperature range of interest right away. It should also cover problematic cases and general conditions on a thermometric experiment.

It is the aim of this short webinar to present some of the basic features of such a theoretical framework for the ratiometric (single ion) luminescent thermometers, which has been recently developed within the NanoTBTEch consortium <sup>[1]</sup>. I will focus on the two key ingredients that dominate the performance of any luminescent thermometer: Thermodynamics, which offers the conditions for optimally working luminescent thermometers, as well as kinetics, which dominates the mechanistic details and often poses limitations to thermometry. The connection between single ion and energy transfer thermometers will be highlighted and what possibilities the theory predicts to overcome apparent limitations to yet achieve a working luminescent thermometer <sup>[2],[3]</sup>.

- [1] M. Suta, A. Meijerink, *Adv. Theory Simul.* **2020**, 3, 2000176, [doi:10.1002/adts.202000176](https://doi.org/10.1002/adts.202000176).
- [2] M. Suta, Z. Antic, V. Dordevic, S. Kuzman, M. D. Dramicanin, A. Meijerink, *Nanomaterials* **2020**, 10, 545, [doi:10.3390/nano10030543](https://doi.org/10.3390/nano10030543).
- [3] T. P. van Swieten, D. Yu, T. Yu, S. J. W. Vonk, M. Suta, Q. Zhang, A. Meijerink, F. T. Rabouw, *Adv. Opt. Mater.* **2020**, 2001518, [doi:10.1002/adom.202001518](https://doi.org/10.1002/adom.202001518).