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Toward a molecular picture of thermophoresis in dilute aqueous solutions

Guillaume Stirnemann*, Alejandro Diaz-Marquez and Mario Araujo-Rocha

[1] *CNRS Laboratoire de Biochimie Théorique, Institut de Biologie Physico-Chimique, PSL University, Université de Paris, 13 rue Pierre et Marie Curie, 75005, Paris, France*
* *stirnemann@ibpc.fr*

ABSTRACT

The emergence of life is one of the most fascinating and yet largely unsolved questions in the natural sciences, and thus a significant challenge for scientists from many disciplines. I will present some of our recent results that specifically address one major issue in the context of life's origins: how to accumulate precursors in abiotic conditions? I will discuss our recent investigation of the poorly-understood thermally-driven process of thermophoresis, which was shown to be an efficient process for the accumulation of dilute precursors in the absence of biological compartments. I will show how our molecular simulations and calculations can shed light on the molecular mechanisms associated with thermodiffusion.

First, I will demonstrate that we can establish a robust simulation set-up to study this problem using non-equilibrium molecular dynamics simulations. I will then show that such simulations lead to results in very good agreement with available experimental data, and previous simulations on model mixtures. We will then see that theories and models that had been suggested in the literature cannot explain thermodiffusion in these solutions, and we will point toward the possible origins for this phenomenon.

REFERENCES

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