On the role of restrained water in biology – muscle contraction as example

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Life has an aqueous origin and consequently all biology on Earth make use of the unique chemical and physical properties of water. There are good reasons why our bodies contains ca 70% water. Dehydrated biomolecules stop quickly working. For example, at normal living conditions for each *gr.* of proteins and nucleic acids, 0.3-0.5 *gr.* of water is required in their hydration shells. Substantial amounts of highly restraint water molecules, with extensively long residence times, can be detected in crystallography and spectroscopy in the closest vicinity of biomolecules. What their eventual functions there are has been a vital area of research in decades. Here we give an example, based on molecular thermodynamics, of the role of restraint water within myosin, and suggest its role in muscle contraction to momentarily store the chemical energy from ATP hydrolysis *as electric energy* before it is converted to mechanical energy in the power stroke by the myosin-actin motor[1] and suggest how to use computational chemistry[2] to study it in more details. This is a topic of debate and there is still no clear consensus of how the large amount of energy provided by ATP is transformed to enable mechanical motion without losing much of it as heat when we use our muscles.

- **References**

[1] *Lampinen M. J. and Noponen T.* Electric dipole theory and thermodynamics of actomyosin molecular motor in muscle contraction. (2005) *Journal of Theoretical Biology* 236, 397–421 DOI: 10.1016/j.jtbi.2005.03.020

[2] *Laaksonen A. and Mocci F.* Molecular Dynamics Simulations and Reaction Rates, in "Comprehensive Computational Chemistry" (Eds. M. Yáñez & R. J. Boyd), Elsevier, 2024, pp. 315-328 https://doi.org/10.1016/B978-0-12-821978-2.00130-6