A dynamic role for water in biological systems

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Received: 11 December 2011 / Accepted: 13 December 2011 /

Published online: 3 February 2012

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Giorgio Careri was consumed by two different ideas about how biomolecules function. He thought that energy transport in proteins was mediated by solitons. Separately, he proposed that protein function was controlled by a network of water molecules, with a density above a critical percolation threshold. He was wrong about the first idea. He was right about the second, but perhaps not quite in the way he imagined it.

The statement that “water is important to biomolecules” is so obvious that it seems pointless to even make it, let alone to set aside a special issue of the *Journal of Biological Physics* on the topic. *Of course* water is important for biological systems. We learned this in elementary school, and this is why scientists searching for life on Mars look for tell-tale evidence of water. What is so great about asserting such a manifestly self-evident statement?

In the field of biological physics, we have only now begun to understand the many marvelously different ways in which water can influence the function of biomolecules. The experimental genesis of these ideas is in the early work of Frauenfelder and collaborators, and in the work of Careri and coworkers. The review by Pascale Mentré [1] in this issue provides a succinct account of the role of water in the orchestration of cell machinery. The review also corrects many misunderstandings. The central ideas are that (i) interfacial water modulates protein function, and (ii) nanoconfined water is so different from bulk water that one cannot simply use the statistical physics models developed for bulk water.

We now also know that there are actually special water molecules that directly participate in protein function. An example of such a special water molecule is in the exciting report on the detection of a special hydrogen-bonded water molecule in the proton pump archaerhodospin-3, by the Rothschild group (Saint Clair et al. [2]). Modern spectroscopic methods continue to advance (see for example the paper on terahertz spectroscopy of water nanoclusters by Johnson [3] in this issue). We expect that this discovery of special water molecules will not be isolated. From an evolutionary point of view, it is logical that some proteins have evolved to take advantage of special water molecules to assist in function, in addition to the interfacial water that inspired Careri.

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The single most exciting addition to the toolkit that is available to biological physicists today involves computational models and methods aimed directly at understanding water. As Fabio Bruni [4] writes in his personal memoir, Careri was singularly uncomfortable with computers. It is therefore interesting that modern computational methods may eventually provide strong support for the role of interfacial nanoconfined water in the functioning of biomolecules. There is not a single accepted computational model of water. The paper by Herzfeld and collaborators [5] describes a tractable and efficient new simulation model for dissociable water in nanoclusters and chains of water. Kumar and Keyes have developed one of the best molecular models for understanding the infrared spectra of water molecules by careful consideration of water in the first hydration shell [6]. Strekalova et al. have studied the effect of a hydrophobic environment, such as one might expect in protein pockets, on a hypothesized critical point in nanoconfined water [7]. The papers suggest the strong vitality inherent in the computational approach, which also provides new insights into the nature of the dynamics of water. One of the most vigorous arguments in the physics of water today involves the nature of the dynamics of water, whether the dynamics are similar to those observed in glassy systems, or whether there is a liquid-critical point. A combination of computational and spectroscopic studies should get us closer to an answer.

Perhaps the most interesting new insight may simply be this: we have known that water is essential for *structure*. It is required for proteins to fold properly. We are now learning that water also strongly influences *dynamics*. New insights based on a combination of novel forms of spectroscopy, data from coherent X-ray sources, computational insights, and new theoretical ideas borrowed from glass transitions and critical phenomena, all have provided firm support to the idea that proteins need to be dynamic in order to function properly, and that protein dynamics are strongly controlled by the dynamic properties of water.

We would like to thank especially our co-editor Feng Wang. Thanks also go to Brigita Urbanc, and to students in Gene Stanley's group at Boston University. We gratefully acknowledge the contributions of the authors of the articles in this special issue, and to the anonymous reviewers who set aside valuable time selflessly. A final thanks to Sonya Bahar, Rudi Podgornik, especially to Maria Bellantone for her inspiration, and to Ruel Pinero and Mieke van der Fluitt for their patience.

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