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一般社団法人日本生物物理学会 第10回 Biophysics and Physicobiology 論文賞受賞講演会  
The 10th Award Seminar for outstanding Biophysics and Physicobiology paper

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オーガナイザー：日本生物物理学会 Biophysics and Physicobiology 論文賞選考委員会

Organizers: Award committee for outstanding Biophysics and Physicobiology paper

日時：11月25日（木）12:10～13:00 / Nov. 25 Thu.

場所：オンライン開催 / Online

形式：講演会 / Lecture

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第10回 Biophysics and Physicobiology 論文賞受賞者

木下正弘

Masahiro Kinoshita

千葉大学大学院理学研究院

Graduate School of Science, Chiba University

蛋白質の折り畳みおよび変性における水の並進配置エントロピーの役割：ブドウ球菌ヌクレアーゼの変異体の熱安定性に関する一理論研究

Roles of translational, configurational entropy of water in protein folding and denaturation: a theoretical study on thermal stability of staphylococcal nuclease mutants

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In general, the structures formed by the biological self-assembly processes are collapsed by the application of high pressures, and the power of forming the structures becomes considerably weaker at low temperatures. In a series of papers [1-4], we have shown that the solute-water many-body correlation component of the translational, configurational entropy of water universally plays critical roles as the driving force in all of these processes. Our theory, where this physical factor is emphasized, is capable of elucidating the pressure [2] and cold [3] denaturation of a protein. Our hybrid of the angle-dependent integral equation theory applied to a molecular model for water and the morphometric approach has been a powerful theoretical method. The Asakura-Oosawa theory, which takes account of only the solute-water pair correlation component, cannot reproduce the pressure and temperature effects described above [4]. In the awarded paper, we investigated the thermal stability of the wild type and nine mutants of staphylococcal nuclease. The thermal stability is correlated not with the number of intramolecular hydrogen bonds, intramolecular electrostatic energy, and area of exposed hydrophobic surface of the protein in the folded state but with the water-entropy gain upon protein folding related to the packing efficiency, core volume, or number of van der Waals contacts of the protein in the folded state.

References: [1] M. Kinoshita, *Biophys. Rev.* 5, 283 (2013); [2] M. Inoue, T. Hayashi, S. Hikiri, M. Ikeguchi, and M. Kinoshita, *J. Chem. Phys.* 152, 065103 (2020); [3] M. Inoue, T. Hayashi, S. Hikiri, M. Ikeguchi, and M. Kinoshita, *J. Mol. Liq.* 317, 114129 (2020); [4] H. Oshima and M. Kinoshita, *J. Chem. Phys.* 142, 145103 (2015).