Abstract Submitted
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Molecular Simulations of Biological Systems under Extreme Conditions YUKO OKAMOTO, Nagoya University — I will present the results of generalized-ensemble simulations of proteins under extreme conditions, namely, high pressure, high temperature, etc. Generalized-ensemble algorithms that we employed were pressure simulated tempering (Y. Mori and Y. Okamoto, J. Phys. Soc. Jpn. 79, 074003 (2010)), multicanonical replica-exchange method (Y. Sugita and Y. Okamoto, Chem. Phys. Lett. 329, 261 (2000)), and replica-exchange umbrella sampling (Y. Sugita, A. Kitao, and Y. Okamoto, J. Chem. Phys. 113, 6042 (2000)). We compare the results with those of experiments.

Yuko Okamoto
Nagoya University

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