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Theoretical Investigations of Biological Nano-Machines

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Protein machines, acting as molecular motors or ion pumps and manipulating other biomolecules, such as DNA, play a fundamental role in living cells. Similar to the machines invented by humans to deal efficiently with the macroscopic world, they contain highly coordinated moving parts[1]. Functional conformational motions in these machines are faithfully repeated in each next operation cycle, despite the fact that such devices are based on soft matter and there are strong fluctuations at microscales. Proceeding from our theoretical studies, I will argue that biological nano-machines correspond to a special kind of proteins selected by evolution[2-4]; I will also discuss how artificial molecular structures with such properties can be in principle designed[2,6].

In our investigations, we use coarse-grained elastic-network models of proteins, whose efficiency is validated by additional full MD simulations6 and by testing their predictions against a set of NMR data for many proteins[7].

1. B. Alberts, Cell 92, 291 (1996)
2. Y. Togashi, A. S. Mikhailov, PNAS 104, 8697 (2007)
3. H. Flechsig, A. S. Mikhailov, PNAS 107, 20875 (2010)
4. Y. Togashi, T. Yanagida, A. S. Mikhailov, PLOS Comput. Biol. 6, e1000814 (2010)
5. A. Sarkar, H. Flechsig, A. S. Mikhailov, New J. Phys. 18, 043006 (2016)
6. L. Dai, H. Flechsig, J. Yu, Biophys. J. 113, 1440 (2017)
7. Y. Dehouck, A. S. Mikhailov, PLOS Comput. Biol. 9, e1003209 (2013)
8. A. S. Mikhailov, *G. Ertl, Chemical Complexity: Self-Organization Processes in Molecular Systems* (Springer, 2017)

9. The figure shows the operation of HCV helicase as conjectured based on single-molecule experiments (left) and reproduced in our structurally-resolved numerical simulations[3].

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