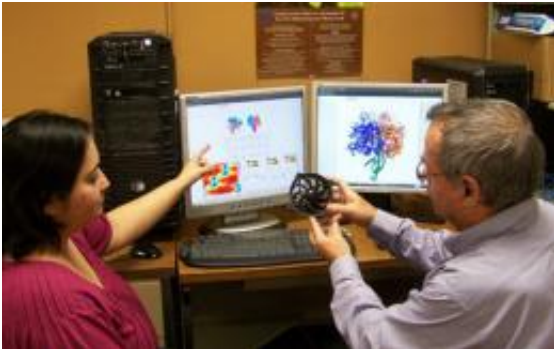


Scientists build working model of life's engine

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Research associate Shayantani Mukherjee and USC Dornsife professor Arie Warshel liken the rotation of F1-ATPase to that of a fan.

(PhysOrg.com) -- Researchers at the University of Southern California have built a theoretical working model of the cellular engine that powers all life.

The [model](#) will allow scientists to better understand the forces of life at the molecular level and potentially replicate them, including designing miniscule mechanical motors for [nanomachines](#) and nanorobots. The work was published online last month in [Proceedings of the National Academy of Sciences](#).

“We were able to take a system that is very complicated and reproduce the crucial action in the system,” said Arie Warshel, Distinguished

Professor of Chemistry and Biochemistry in USC Dornsife. “We still have a lot of questions, but this is clearly a large step toward understanding the action of such ubiquitous engines in living systems.”

The body’s cellular engine is a protein molecule whose rotation generates the universal “fuel” — adenosine triphosphate (ATP) — that powers processes in living cells. The 1997 Nobel Prize in Chemistry was awarded to the scientists who elucidated the structure of this protein and outlined the principles of how it may operate.

The protein rotates, drawing in raw materials and synthesizing them into ATP. This fuel-generating engine can be divided into two parts, one of which is a rotating piece called F1-ATPase.

Warshel and research associate Shayantani Mukherjee built a computer-generated model of F1-ATPase that was remarkably successful at replicating the essential physical forces underlying the workings of the engine, mirroring the cellular motor’s unique unidirectional rotation.

Previous attempts to build such models relied on complex systems in which every atom was represented — making it difficult to determine why the motor is working, Warshel said.

Instead, Warshel and Mukherjee took a bare-bones approach, simplifying the structure — a strategy known in the computational biology world as “coarse-graining.”

“Make everything as simple as possible, but not simpler,” Warshel said.

Their simplified model rotated in the same manner as F1-ATPase, even pausing at exactly the same places. It also provided the clearest description yet of how the chemical energy of the ATP is used to rotate the motor and why the motor actually works.

Provided by University of Southern California

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