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Kinesin molecular motor as an electrostatic machine

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Kinesin is a two-headed motor protein that uses ATP hydrolysis to propel itself on tubulin microtubules advancing in 8nm discrete steps.[1] Two decades of experiments and modeling have shed light on many biological, physical and chemical details on molecular motor's phenomenology, but a deep picture of the physical processes controlling its processivity, bidirectionality and the conversion of chemical energy into mechanical work is still lacking. We show here through numerical calculation of the involved electro-chemical phenomena that some of the accepted experimental features, also the most recent, can be explained by considering that kinesin is an electrostatic motor. Utilizing electric charge distributions fixed on microtubules and ATP dependent charges being on kinesin heads we obtain a set of coordinate rotations and translations that leads to a step-like motion along the protofilament. We find that it is not necessary to assume global conformational changes. Our calculations lead to a global movement induced by Coulomb forces within the Debye screening range and volume exclusion domains. This specific directional motion is made possible by two symmetry breaking physical processes related to the net electric polarity of tubulin [2] and to the fact that the amino-acidic character of the stalk domain provides a specific charge to the neck. Our calculations show that the net microtubule dipole moment as well as the neck charge determines whether the motor is plus (wild-type) or minus-ended (ncd). The three-dimensional electric field induced by the tubulin dipole moment forces the motor to walk parallel to a protofilament. Additionally, our calculations imply that processivity is linked to the existence of substeps, a fact that can stimulate new experiments.

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[1] Visscher,K., Schnitzer,M.J., & Block,S.M. "Single kinesin molecules studied with a molecular force clamp". *Nature* **400**, 184-189 (1999).

[2] Tuszynski,J.A.,Luchko,T.,Carpenter,E.J. & Crawford,E. "Electrostatic Properties of Tubulin and Their Consequences for Microtubules." *J.Comput.Theor. Nanosci.* **1**, 4 (2005).