

Manubot Rootstock: Molecular motors with barriers

Authors

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Abstract

TBD

Outline

1. Surface with and without a barrier
2. Family of curves showing force on the barrier as a function of height and position of the barrier.
3. Optimization of a surface for flux and force with and without a barrier. [\[1\]](#)

Ideas

1. MD and umbrella sampling of a Feringa-type motor.
 2. pH change can be modeled as a change in substrate concentration, for our purposes.
 3. Can the experimental groups synthesize motors based on an energy surface?
 4. CD can be a platform -- a scaffold -- for building, but it will be hard to figure out the appropriate assays.
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1. Slochower DR, Wang Y-H, Tourdot RW, Radhakrishnan R, Janmey PA. 2014 Counterion-mediated pattern formation in membranes containing

anionic lipids. *Advances in Colloid and Interface Science***208**, 177–188.
See <https://doi.org/10.1016/j.cis.2014.01.016>.