## Manubot Rootstock: nonequilibriumbarrier

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# Manubot Rootstock: Molecular motors with barriers

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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.
- 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 <a href="https://doi.org/10.1016/j.cis.2014.01.016">https://doi.org/10.1016/j.cis.2014.01.016</a>.