

Computational Biology Seminar 2/27 - Jane Shen

"Proton-Coupled Biological Ion and Substrate Transport: Insights from constant pH Molecular Dynamics"

- K-MD is this like free energy perturbation?
- ↳ proton steps bonded, just has the force to pretend it isn't there.
- ↳ this is literally free-energy perturbation, but centered around pH
- ↳ use replica-exchange, in pH or temperature space.
- I should read about lipids
- ↳ woman that she seems to know keeps interrupting her.
- ↳ "microscopy" -- definitely learned that in Germany.
- ↳ "Poisson-Boltzmann" calculations
- ↳ this seems like it works decently well. I should read one of her papers
- ↳ essentially looking at pH controlled allostery.
- ↳ polarizable force field would really help this method.