Physical & Quantitative Biology, BME/CHE/PHY 558

Fall 2022 – Mon, Wed, Fri, 10:30 – 11:25 AM, in Laufer Center Room 101.
Recitations: Mon, 11:30 am – 12:30 pm in Laufer Center Room 101.

Course goals: The central idea of this course is the free energy, the quantitative way we understand thermodynamic forces driving the equilibria and transition rates in chemistry, physics and biology. We describe the components underpinning free energy: the entropy and internal energy. We explore the microscopic interactions - including hydrogen bonding, van der Waals interactions, electrostatics and hydrophobic forces - that explain physical and chemical mechanisms in cell biology and are the workhorse tools in computational drug discovery. We show how these basic ideas are applied: binding affinities form the basis for synthetic biology and drug discovery; coupled binding explains how biological machines convert energy and transduce signals or control gene activity; and polymer free energies form the basis for the folding of protein and RNA molecules; with implications for molecular and cellular evolution.

Textbook: Molecular Driving Forces by Dill & Bromberg. Garland Science, 2010
Textbook: Protein Actions by Bahar, Jernigan & Dill. Garland Science, 2017
Extra textbook: Physical Models of Living Systems by Nelson. W. H. Freeman & Co., 2015

#1: 8/22) Introduction. Basic Biology. Probability, statistics. (MDF 1,2) [GB]
#2: 8/24) Combinatorics. Distributions. Extremum principles. (MDF 2, 3) [GB].
#3: 8/26) Energy and Multiplicity. Thermo laws. Multivariate calculus. (MDF 4) [GB].

#4: 8/29) Multivariate Optimization. Max Ent & Boltzmann principle. (MDF 5) [GB]. **TA: JP.**
#5: 8/31) Energy vs. Entropy formulation. Thermo states. (MDF 6) [GB].
#6: 9/2) Driving forces. Path integrals. (MDF 6,7) [GB].

9/5) **NO CLASS**, Labor Day.
#7: 9/7) Ideal gas. Carnot cycle. (MDF 7) [GB]. **TA: JP.**
#8: 9/9) Free energies. Maxwell relations. (MDF 8,9) [GB].

#9: 9/12) Susceptibilities. Boltzmann Law. (MDF 9,10). [GB] **TA: JP.**
#10: 9/14) Partition function. Simple gases, solids. (MDF 10,11). [GB]
#11: 9/16) Chemical equilibria. (MDF 12,13) [GB].

#12: 9/19) Liquids, phase equilibria. Mixtures. (MDF 14,15) [GB]. **TA: JP.**
#13: 9/21) Solvation. (MDF 16) [GB].
#14: 9/23) Diffusion, Fick's Law. Random walks. Time's arrow. (MDF 17,18). [GB].

#15: 9/26) Chemical rates. Mass-action kinetics. Transition states. (MDF 19). [GB]. **TA: JP.**
#16: 9/28) Coulomb & electrostatics: charges, potentials, fields. (MDF 20,21). [GB].
#17: 9/30) Electrochemical equilibria. Batteries. (MDF 22) [GB].

#18: 10/3) Salts+charges. Poisson-Boltzmann. Intermolec. forces. (MDF 23,24) [GB]. **TA: JP.**
#19: 10/5) Real gas. Phase transitions. Adsorption & binding. (MDF 24,25) [GB].
10/7) **MIDTERM EXAM 1**.

10/10) **NO CLASS**, Fall Break.
#20: 10/12) Michaelis-Menten. Catalysis. Cooperativity. (MDF 27,28) [GB]. **TA: CK.**
#21: 10/14) Bio-machine principles. (MDF 29) [GB].

#22: 10/17) Water: pure and as a solvent. (MDF 30, 31) [MFernandez-Serra]. **TA: CK.**
#23: 10/19) Polymers 1: Conformations. Random flights. (MDF 33, 34) [HStrey].
#24: 10/21) Polymers 2: Solutions, Flory-Huggins. (MDF 32,33) [HStrey].

#25: 10/24) Protein structures. (PA1) [MS or CS]. **TA: CK.**
#26: 10/26) Protein function & mechanisms. (PA2) [MS or CS].
#27: 10/28) Protein folding & stability. (PA3)[CS].

#28: 10/31) Cooperativity in proteins. (PA5)[CS]. **TA: CK.**
#29 11/2) Protein folding on energy landscapes. Aggregation. (PA6) [RRazban].
#30: 11/4) Protein evolution and sequence space. (PA7) [JRest].

#31: 11/7) Bioinformatics. (PA8) [DKempa]. **TA: CK.**
#32: 11/9) Gene expression and its regulation. [GB].
#33: 11/11) Natural and synthetic gene networks. [GB].

#34: 11/14). Drug discovery & methods. [DKozakov]. **TA: CK.**
#35: 11/16) Drug discovery in industry. [JVD].
11/18) Research Project Presentations.

11/21) **MIDTERM EXAM 2**.
11/23) **NO CLASS,** Thanksgiving break.
11/25) **NO CLASS,** Thanksgiving break.

MDF = Molecular Driving Forces, chapter numbers. PA = Protein Actions, chapter numbers.
TAs: Jonathan Pachter (JP), Charles Kocher (CK).

Lecturers
[GB] Gábor Balázsi
[DKozakov] Dima Kozakov
[DKempa] Dominik Kempa
[RRazban] Rostam Razban
[CS] Carlos Simmerling
[MFS] Marivi Fernandez-Serra
[JRest] Joshua Rest
[MS] Markus Seeliger
[HStrey] Helmut Strey
[JVD] John H. Van Drie

All lectures & recitations will be recorded and links posted later on Blackboard.

Student Accessibility Support Center Statement
If you have a physical, psychological, medical, or learning disability that may impact your course work, please contact the Student Accessibility Support Center, 128 ECC Building, (631) 632-6748, or via e-mail at: **sasc@stonybrook.edu**. They will determine with you what accommodations are necessary and appropriate. All information and documentation is confidential.

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