Project Ideas and References

1. Liquids and Gases

- Polyatomic gases
- Cluster expansion, Cluster diagrams
- Virial equation of state
- Liquid state theory, correlation functions, perturbation theory of liquids, Kirkwood-Buff theory, classical density functional theory
 - o https://en.wikipedia.org/wiki/Kirkwood%E2%80%93Buff_solution_theory

2. Materials and Phase Behavior

- Ising model (most simple model of a phase transition)
- Landau theory (field theory of phase transitions)
 - o https://en.wikipedia.org/wiki/Landau_theory
- Einstein crystal (heat capacity of solids)
- Scaling theory and renormalization group theory

3. Chemical Kinetics

- Chemical Equilibrium
- Stochastic Reaction Kinetics (fluctuation effects in chemical reactions)

4. Non-equilibrium/Transport

- Chapman-Enskog Theory (prediction of transport coefficients)
- Boltzmann Equation, Kinetic Theory, BBGKY Heirarchy (nonequilibrium statistical mechanics of gases)
 - o <u>https://en.wikipedia.org/wiki/Boltzmann_equation</u>
 - o https://en.wikipedia.org/wiki/BBGKY_hierarchy

- Langevin Equations and Brownian Motion (nonequilibrium statistical mechanics most relevant for bio, polymers, colloids, etc.)
- Fokker-Planck equations and Master equations
- Fluctuation-Dissipation Theorem (connection between friction and diffusion)
- Time-correlation functions and Green-Kubo relations
 - o https://en.wikipedia.org/wiki/Green%E2%80%93Kubo_relations
 - o https://en.wikipedia.org/wiki/Correlation_function_(statistical_mechanics)

5. Soft Materials

- DLVO Theory (interactions between colloids)
 - o https://en.wikipedia.org/wiki/DLVO_theory
- Flory-Huggins Theory (mixing thermodynamics of polymer solutions and melts)
- Statistical Thermodynamics of ideal polymer chains (radius of gyration, osmotic pressure, etc)
- Statistical field theories of polymers

6. Electrolytes

- Debye-Hückel Theory (double layers in electrolytes), generalization of D-H Theory to Poisson-Boltzmann theory
- Counterion/Manning Condensation
 - o <u>https://doi.org/10.1063/1.1672157</u>
 - o <u>https://doi.org/10.1137/0146061</u>
- Bjerrum Association
 - o https://en.wikipedia.org/wiki/Bjerrum_length
 - Côté, JF., Perron, G. & Desnoyers, J.E. Application of the Bjerrum Association Model to Electrolyte Solutions. III. Temperature and Pressure Dependencies of Association Constants. *Journal of Solution Chemistry* 27, 707–718 (1998). https://doi.org/10.1023/A:1022653506593

- (Harder) Concentrated electrolytes, molten salts and ionic liquids
 - o Coulomb gas: <u>https://en.wikipedia.org/wiki/Coulomb_gas</u>
 - Coulomb fluids:
 - This perspective looks fantastic: "Perspective: Coulomb fluids—Weak coupling, strong coupling, in between and beyond", <u>https://doi.org/10.1063/1.4824681</u>
 - Liquid metals, molten alts, and ionic liquids https://link.springer.com/chapter/10.1007/978-3-642-17779-8_2
 - Size and/or charge asymmetry effects in coulombic fluids in the presence of external fields: From simple electrolytes to molten salts, <u>https://doi.org/10.1016/j.bpc.2021.106747</u>
 - Molten Salts From Fundamentals to Applications, https://link.springer.com/book/10.1007/978-94-010-0458-9
 - https://www.taylorfrancis.com/chapters/edit/10.1201/9781351069472-2/introduction-statistical-mechanics-solutions-robert-mazo
 - List of open problems and some good references: <u>https://www.cecam.org/workshop-details/electrostatics-in-concentrated-</u> <u>electrolytes-294</u>
 - Recent work by Zhen-Gang Wang (a deeply thinking theorist)
 - https://www.worldscientific.com/doi/abs/10.1142/S0219633608003824
 - Fluctuation in electrolyte solutions: The self energy, https://doi.org/10.1103/PhysRevE.81.021501
 - Effects of image charges on double layer structure and forces, <u>https://doi.org/10.1063/1.4821636</u>. A good overview of the state of Poisson-Boltzmann theory in the introduction.
 - Electrostatic correlations and the polyelectrolyte self energy, https://doi.org/10.1063/1.4975777
 - On the theoretical description of weakly charged surfaces, <u>https://doi.org/10.1063/1.4914170</u>. Good description of the limitations of Poisson-Boltzmann theory.

- Inhomogeneous screening near the dielectric interface, https://doi.org/10.1063/1.4945011
- Work by <u>Fyl Pincus</u> (another important theorist, more of his work is on polyelectrolytes)
 - Scaling perspectives of underscreening in concentrated electrolyte solutions, <u>10.1039/D3SM01094E</u>
 - Electrolyte and polyelectrolyte solutions: limitations of scaling laws, osmotic compressibility and thermoelectric power. <u>https://doi.org/10.1016/0032-3861(80)90268-2</u>
 - Debye Length and Double-Layer Forces in Polyelectrolyte Solutions, https://doi.org/10.1021/ma011893y
 - Attractions between Like-Charged Surfaces with Dumbbell-Shaped Counterions, <u>https://doi.org/10.1103/PhysRevLett.101.208305</u>
 - Electrolytic depletion interactions,
 <u>https://doi.org/10.1103/PhysRevE.60.6549</u>

7. Special Topics

• Fermi-Dirac or Bose-Einstein statistics/gases (quantum gases)