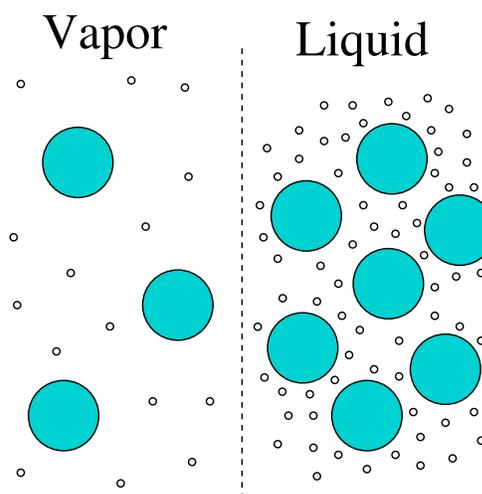


Theoretical and Computational Studies of Macromolecular Materials

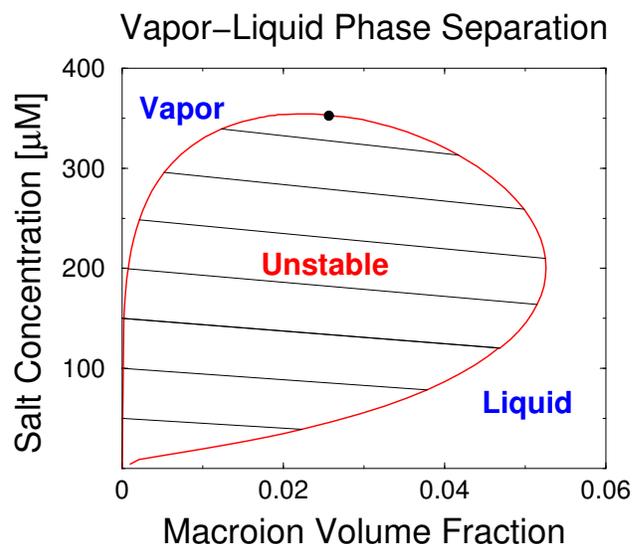
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Colloidal suspensions consist of mesoscopic particles, smaller in diameter than the width of a human hair, suspended in a liquid. Familiar examples are paints, inks, clays, milk, and blood. Beyond traditional applications in the chemical, mining, food, and pharmaceuticals industries, colloidal materials play a key role in emerging nanotechnologies. Because of their unique optical and thermal properties, colloidal crystals are a basis for fast optical switches, chemical sensors, and photonic bandgap materials, while DNA-coated particles have potential for drug delivery.

Designing and fabricating novel materials requires fundamental understanding of microscopic interactions. Here we present results from computational modeling of electrically charged colloidal particles (macroions) suspended in water. For highly charged particles, electrostatic interactions can profoundly influence large-scale behavior, even driving the system to separate into dilute (vapor) and concentrated (liquid) phases at low salt concentrations.



Charged colloidal macroions (large spheres) and microions (small spheres) can be driven by electrostatic interactions to separate into colloid-poor (vapor) and -rich (liquid) phases.



Phase diagram, showing boundary of region (red) within which a colloidal suspension, at specified macroion and salt concentrations, is unstable toward vapor-liquid separation.

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Education

Two graduate students (Ben Lu and Shrikant Shenoy) and one postdoctoral fellow (Hao Wang) are contributing to this work. Lu and Shenoy are Ph. D. candidates, who are receiving training, and acquiring expertise, in applying computational methods to modeling soft materials. They have presented results on colloidal suspensions at two scientific conferences. Wang recently joined the group and will present results on polyelectrolyte solutions at an upcoming international conference.

The PI has given presentations on soft materials to several student groups, has facilitated at the North Dakota Science Olympiad, and has been a judge at two state science fairs for high school and junior high school students. He is involved in implementing an online learning network for use in introductory Physics classes at NDSU and for outreach to local and regional high schools.