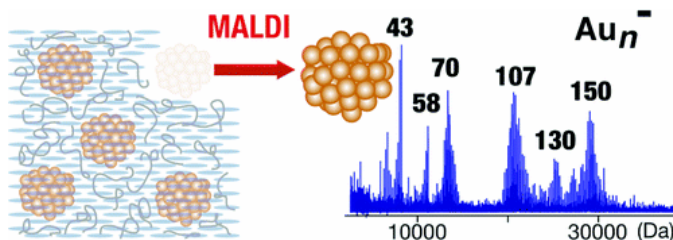


Physical Chemistry Cume
Petr Kral
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In this cume, you can show how well you understand some thermodynamics and electrostatics.

1. In the figure (right), you can see the mass spectrum of gold clusters stabilized in poly(vinyl-pyrrolidone) (JACS 131, 18216 (2009)).



a) Why do you think that only certain masses of clusters are predominantly observed?

b) How would you understand the concept of surface energy of the gold cluster? Can it lead to a pressure change inside the cluster? (explain). Can the cluster shape depend on the temperature?

c) Imagine that you leave colloidal gold cluster to self-assemble in a nonpolar solvent. What do you think are the important forces between the particles that determine their self-assembly? What lattice will they form? How would you propose to control the inter-particle forces to change the structures formed? (Use formulas in your explanations).

d) Imagine that you have C_{60} molecules in a gas phase and you slowly cool the gas down. What do you expect will happen to the gas? Is it similar as in water vapor? (Hint: think about the extent of coupling forces between the components and the size of the components).

e) Imagine that you have biological membrane in ionic solution where some of the lipids in the membrane are charged (+) and you let adsorb on it a linear polymer with oppositely charged groups (-) separated by certain distances along its length. Do you think that the desorption rate of the linear polymer from the membrane depend on the distances of its charged group? Why?

2. Imagine that you have an ionic solution of oppositely charged and hydrated ions.

a) What is the character of the electrostatic field around a selected ion in this system? (Explain and describe by formula).

b) Imagine that you form from this solution a neutral droplet and add a single ion in its center. What will be the electric field generated by this ion inside and outside the droplet, which is assumed to be in vacuum? Does it depend on the droplet size? How?

c) Assume now that you put the droplet in b) inside a spherical gold shell (closed) of the internal radius r and thickness d . What will be the electric field in the gold and outside the gold shell?

3. In the figures shown below you can see snapshots of molecular dynamics simulations done for water in a box (no gravity). From the initial nonequilibrium state at 400 K (1), some clusters are formed (2). The system is then cooled to 300 K (3) and finally brought to the critical temperature (4). You can assume, for simplicity, that the snapshots 2, 3 and 4 (not 1) are taken in equilibrium.

a) Why does the system evolve from 1 to 2? What would be the evolution if the same amount of molecules was in twice smaller box at the same T? What happens to the pressure when the volume changes as described?

b) What does control the number of lonely molecules in 2? What are the chemical potentials in the system? Why are some water molecules still seen alone in 3? Can you get rid of them if you wait long enough? (Explain)

