

Phase diagram of two dimensional colloids : implications for membrane protein organization

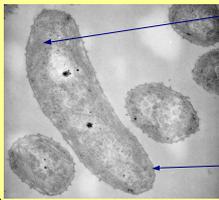
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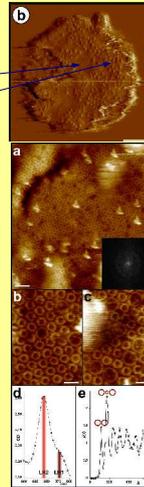
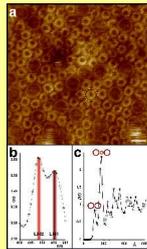
Organization of Bacterial Photosynthetic Membranes

Recently high resolution AFM images have revealed the organization of proteins in bacterial photosynthetic membranes. The organization revealed is remarkable and all the more so when we realise that these protein rich membranes develop from lipid rich cytoplasmic membranes.



Intracytoplasmic photosynthetic membranes are specialized membranes that contain the proteins of the photosynthetic apparatus and little else. The cytoplasmic membrane surrounds the cell.

Intracytoplasmic photosynthetic membranes show long range order (LH2 rich and core complex rich). High resolution images shows addition of LH2 does not push the core complexes apart!!



Core complex neighbors (7 on average)...

LH2:LH1	7	3.5
0(LH1)	44	50
1(LH1)	40	36
2(LH1)	15	14
$p(LH1) = 0.105$ $p(LH2) = 0.895$		
LH2 in crystals ...		
LH2:LH1	7	3.5
% LH2 in crystals	50	5
LH2 _{NC} :LH1	3.5	3.3

Rules of organization

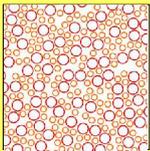
There is a constant mixture of about 3.5 LH2/core complex in a disordered state.

The excess LH2 is present in 2 dimensional hexagonally packed crystals

In the disordered mixture each core complex is 8.5 times more likely to have LH2 neighbors rather than core complex neighbors.

Modeling Photosynthetic Membrane Development

To model the development of this membrane system we treated the membrane as a plane and the proteins as colloidal discs that can diffuse in the plane of the membrane. The interactions between the proteins are then defined by a potential. We used a Kihara type potential for the different interactions. This potential is characterised by 4 parameters for each interaction (a, σ , d, and ϵ). We used for these values: σ measured

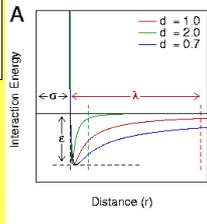


$$U(r) = \begin{cases} \infty & r \leq a \\ 4\epsilon \left[\left(\frac{\sigma-a}{r-a} \right)^{12} - \left(\frac{\sigma-a}{r-a} \right)^6 \right] & r > a \end{cases}$$

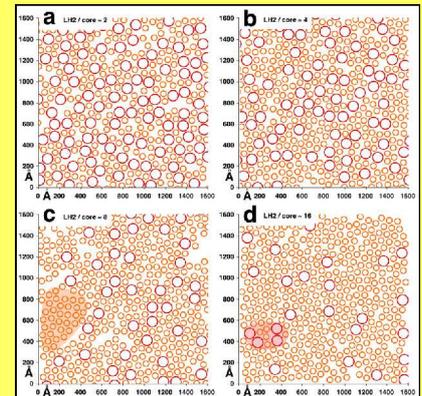
Interaction forces	
LH1	LH2
2	5
5	3

from AFM, 'a' was arbitrarily set to 0.2nm less than σ . The well depths were set using the observed statistical preferences.

Using a Monte-Carlo Gibbs ensemble approach we were able to mimic the separation of "protein rich" membrane regions from "protein poor" membrane regions and obtain native-like organization of the different sized rings in the "protein rich" domains. This success was dependent on relatively long distance interactions (d=1.0 gave good results).



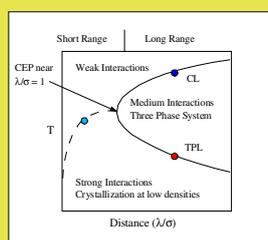
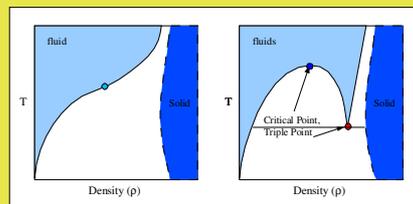
Modeled organization of "protein rich" regions for different compositions.



General Model of Membrane Protein Self-Organization

To model the development of this membrane system more generally we have examined the phase diagram of 2 dimensional colloidal discs using NPT, NVT and Gibbs ensemble Monte-Carlo simulations. The Kihara potential conveniently separates interaction distance, length scale and interaction energy.

- For short range interactions there are 2 phases a fluid and a solid phase.
- For long range interactions there is the appearance of a second fluid phase and associated critical and triple points.
- The projection of the three-dimensional (T/ ρ / λ) phase diagram onto the T/ λ plane shows the separation of the diagram into long and short range domains and strong/medium and weak strength domains.



Conclusions

Complex phase behavior depends on medium intensity long range interactions. The necessity for long range (with respect to object size) suggests that electrostatic interactions, membrane elastic deformations and lipophobic effects could be particularly important.

The parameters that we work in modeling membrane development for interaction strength and distance of interaction are those of medium strength – long range interactions.

Bibliography

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 Scheuring, Sturgis, Prima, Bernadac, Levy and Rigaud (2004) *Proc.Nat.Acad.Sci* **31**: 11293-11297.