

Polymorphism in Lattice Models



What is polymorphism?

Why are the clues?

Simpleste Model for Polymorphism?

Summary

Our Group



What is polymorphism? Chicken



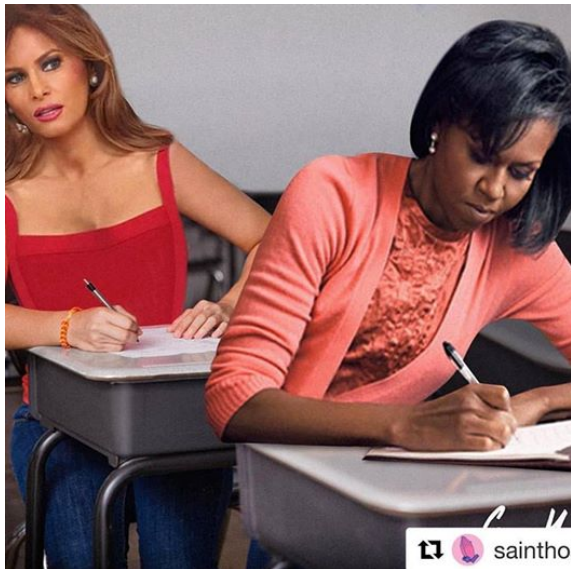
What is polymorphism? Birds



What is polymorphism? Snail



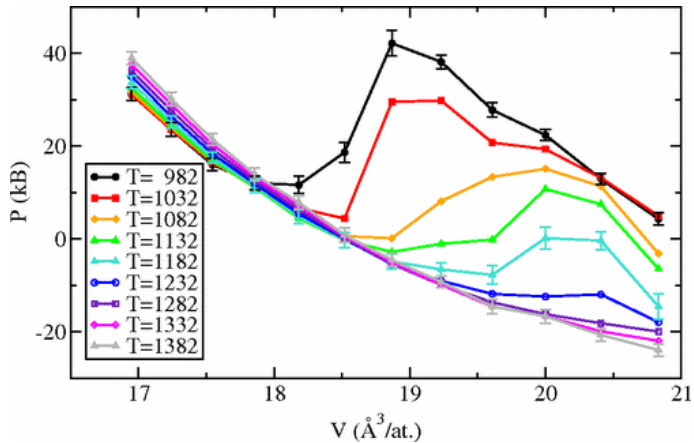
What is polymorphism? President's wife



  sainttho

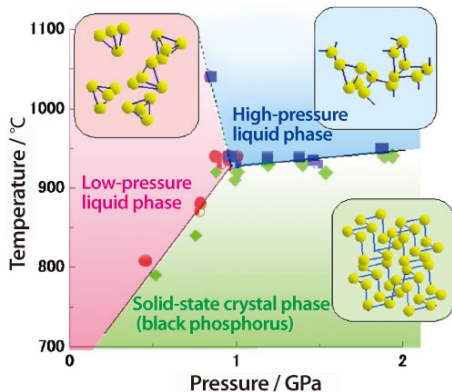
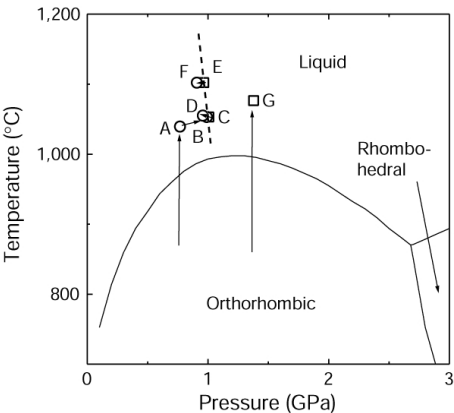
What is polymorphism? Silicon

Ganesh and Widom, PRL 102, 075701 (2009)

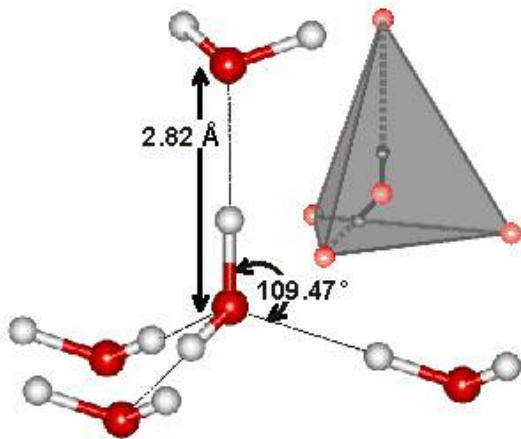


What is polymorphism? Phosphorus

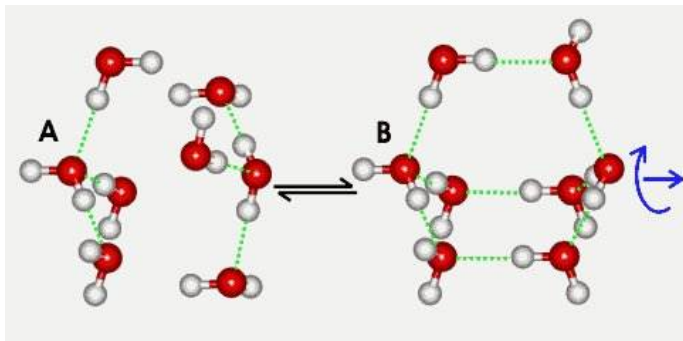
Katayama et al, Nature 403, 170(2000)



Water



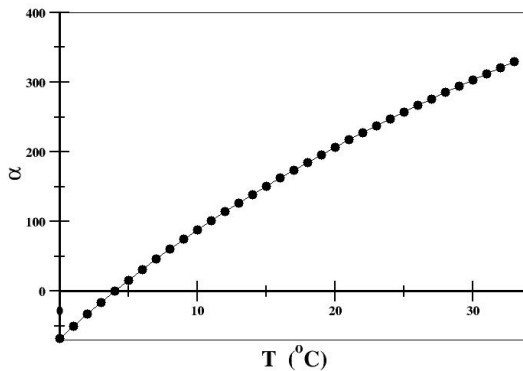
Two Structures



Thermal Expansion

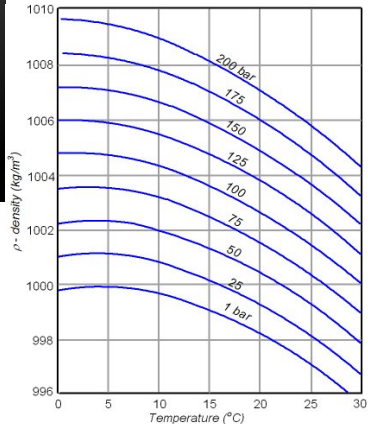
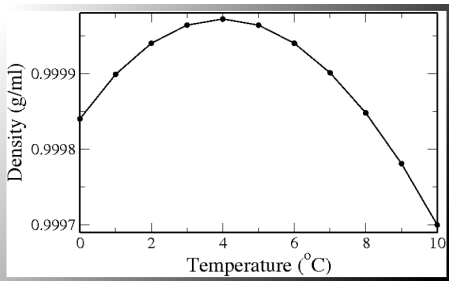
Kell, J. Chem. Eng. Data 20, 97 (75)

$$\alpha_P = \frac{1}{V} \left\{ \frac{\partial V}{\partial T} \right\}_P$$



Density

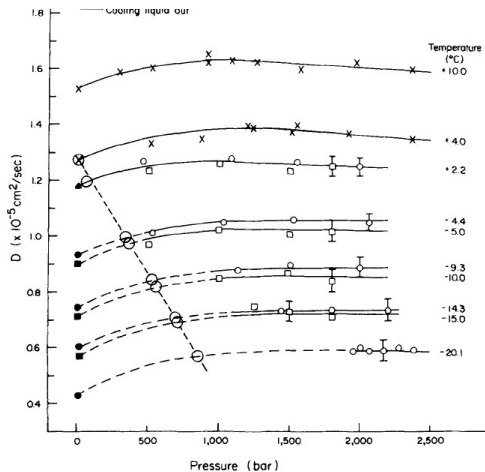
Kell, J. Chem. Eng. Data 12, 66 (67)



Diffusion

Angell, Finch, Bach 65, 3063 (76)

► $\langle r(t)r(0) \rangle = 6Dt$



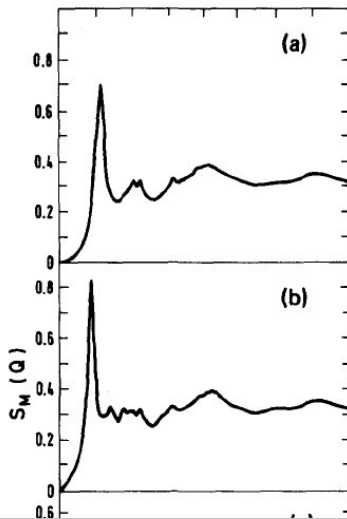
Spoiler Alert

Stanley's Lecture



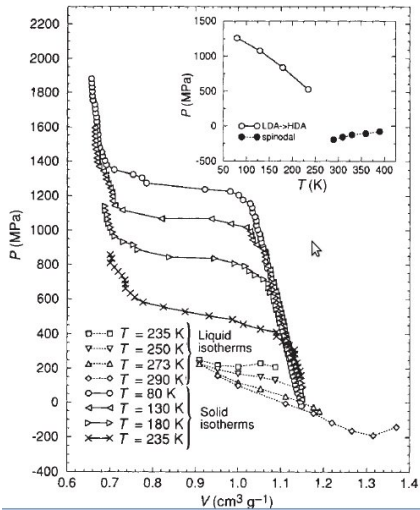
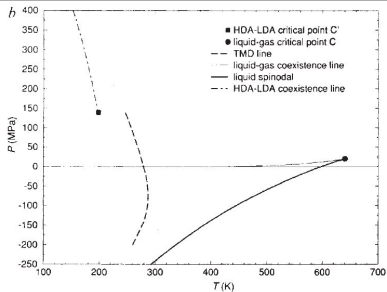
Fases Amorfas

Belliscent-Funel, Teixeira, Bosio, JCP 87, 2231 (87)



Liquid-Liquid Phases

Poole, Sciortino, Essmann, Stanley, Nature 360, 324 (92)



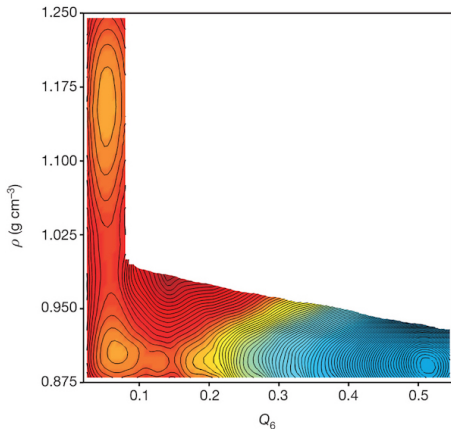
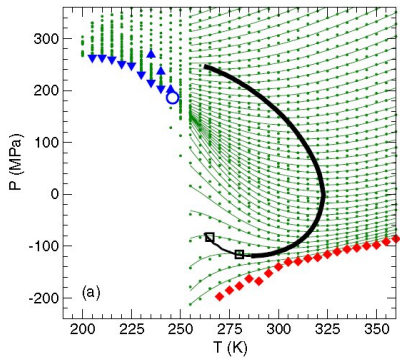
Spoiler Alert

Stanley's and DeBenedetti's Lecture



ST2

Stanley's and Debenedetti's Lecture

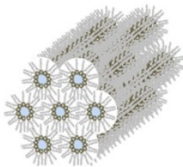


What are the clues? Amphiphilic

MGDG, MGlcDG,
PE, PS, PA, DPG



HII phase



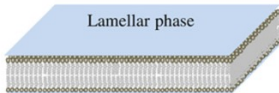
Cubic phase



DGDG, DGlcDG,
SQDG, PC, PG, PI



Lamellar phase

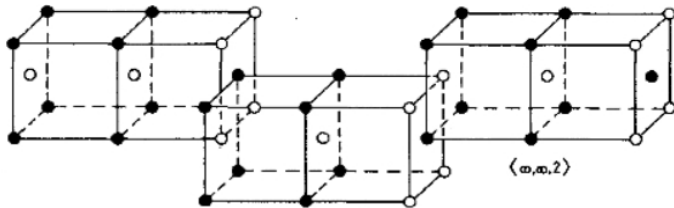


Lysolipid

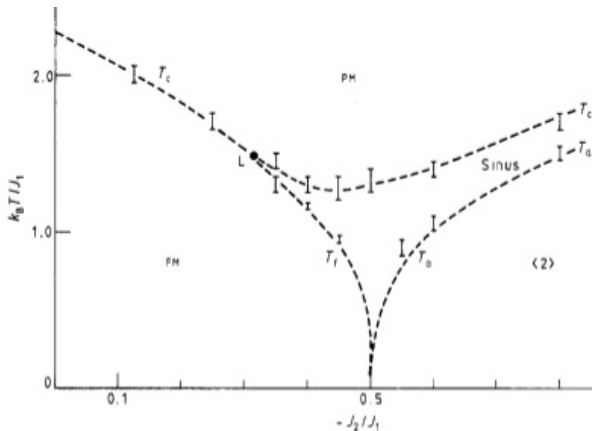


HI phase

What are the clues? Amphiphilic
MCB, Phys. Rev. B 42, 6363 (1990)

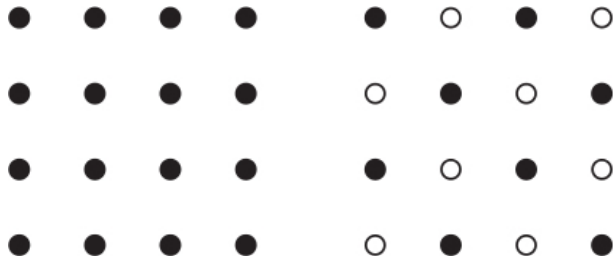


What are the clues? Amphiphilic MCB, Phys. Rev. B 42, 6363 (1990)



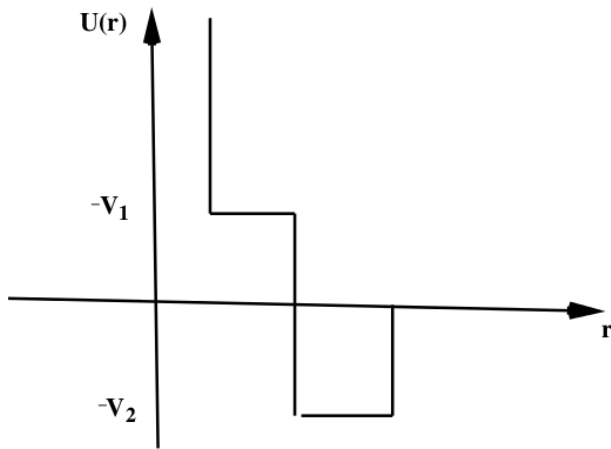
Simplest Model for Polymorphism? 2d Lattice

Balladares and MCB, JPCM 16, 8811 (2014)



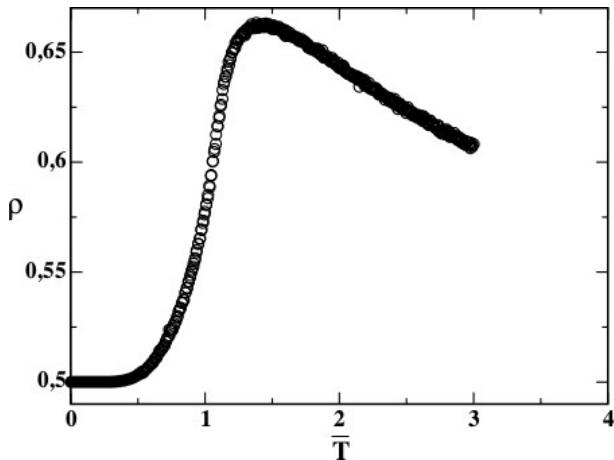
Simplest Model for Polymorphism? Potential

Balladares and MCB, JPCM 16, 8811 (2014)



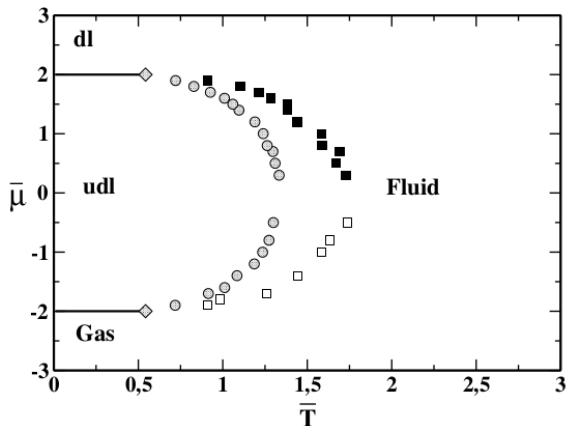
Simplest Model for Polymorphism? Density Anomaly

Balladares and MCB, JPCM 16, 8811 (2014)



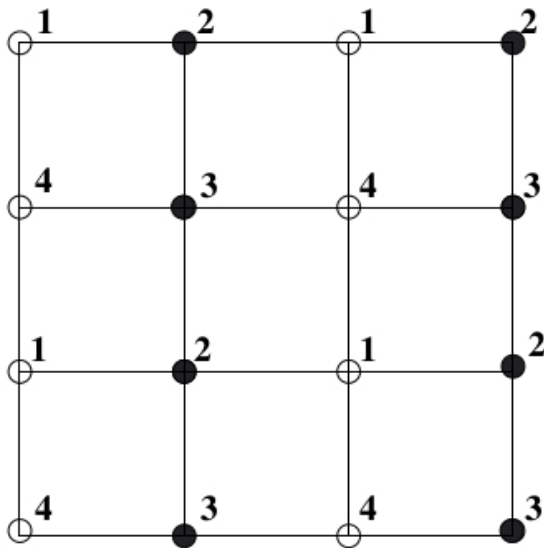
Simplest Model for Polymorphism? Phase Diagram

Balladares and MCB, JPCM 16, 8811 (2014)



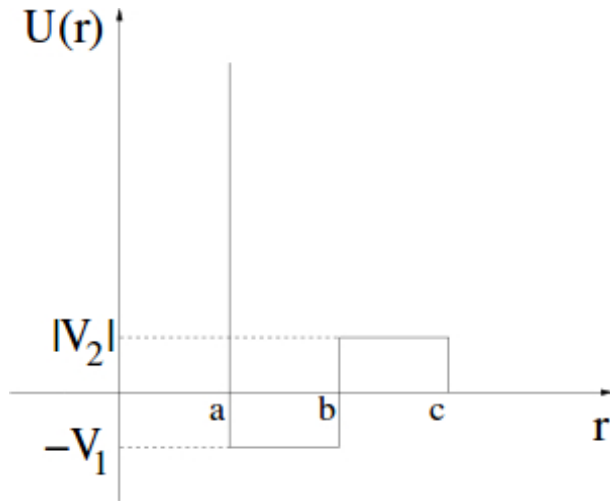
Simplest Model for Polymorphism? 2d Lattice

de Oliveira, MCB, JPCM 17, 399 (2005)



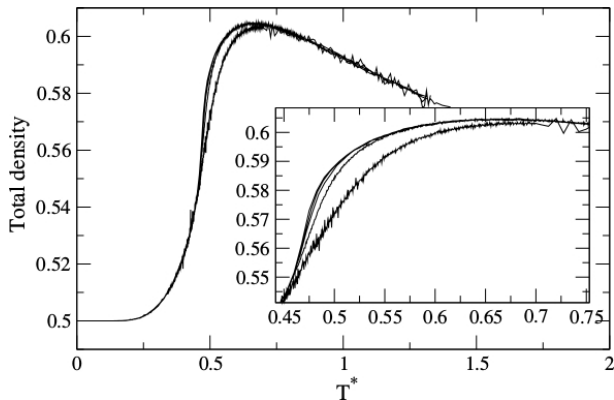
Simplest Model for Polymorphism? Potential

de Oliveira, MCB, JPCM 17, 399 (2005)



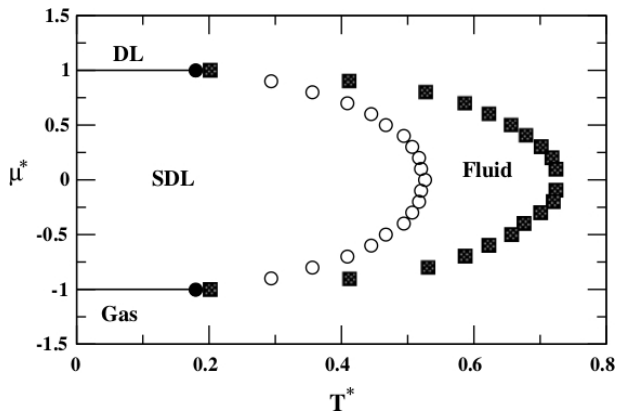
Simplest Model for Polymorphism? Density

de Oliveira, MCB, JPCM 17, 399 (2005)



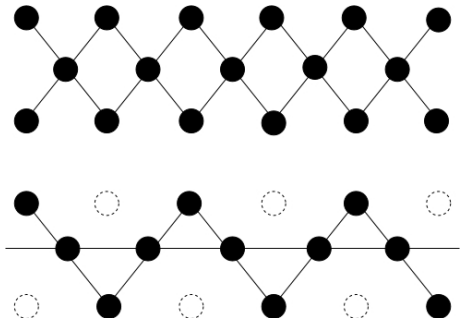
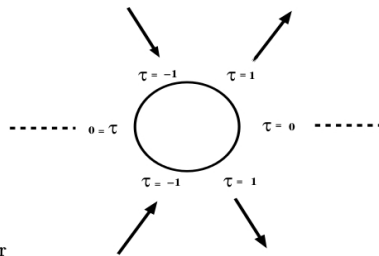
Simplest Model for Polymorphism? Phase Diagram

de Oliveira, MCB, JPCM 17, 399 (2005)



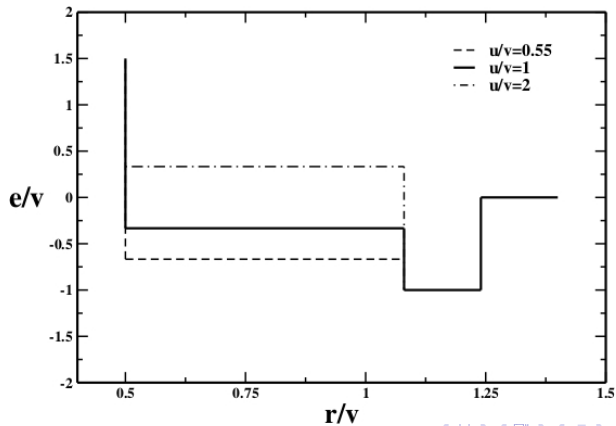
Simplest Model for Polymorphism? 2d Associating Lattice Gas

Henriques and Barbosa, PRE 71, 031504(2005)



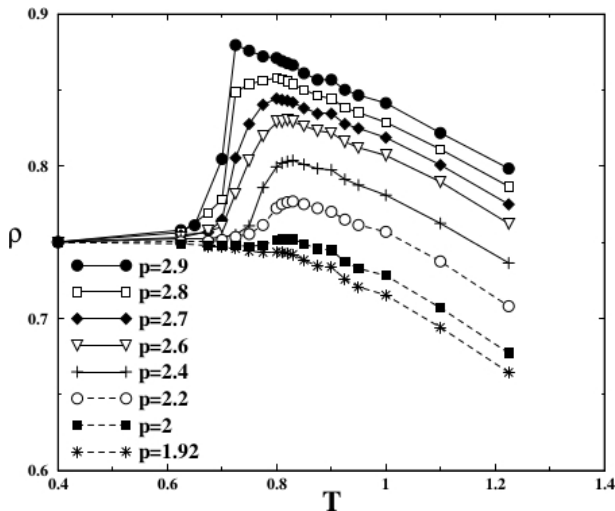
Simplest Model for Polymorphism? Potential

Henriques and MCB, PRE 71, 031504(2005)



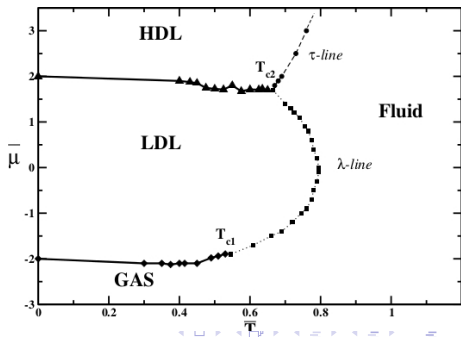
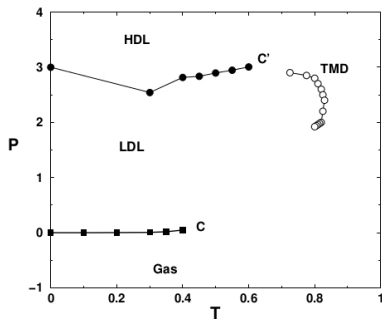
Simplest Model for Polymorphism? Density

Henriques, MCB, PRE 71, 031504 (2005)



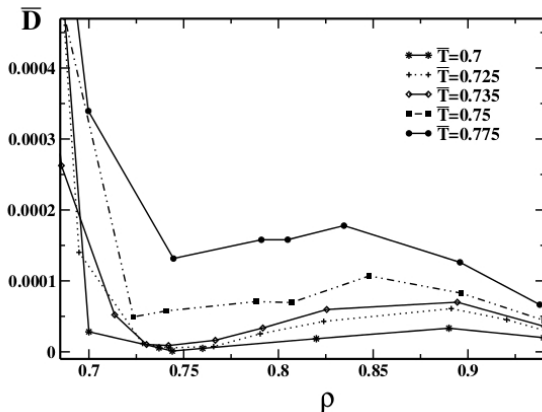
Simplest Model for Polymorphism? Phase Diagram

Girardi, Szortyka, Henriques and MCB, JCP 130, 184902 (2009)



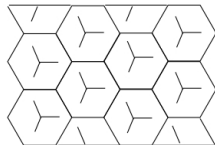
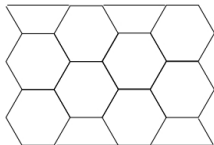
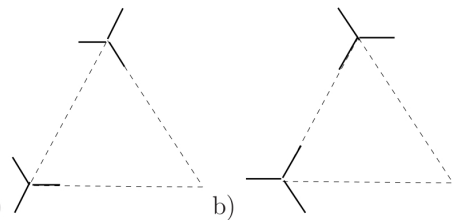
Simplest Model for Polymorphism? Diffusion

Physica A 386 692 (2007)



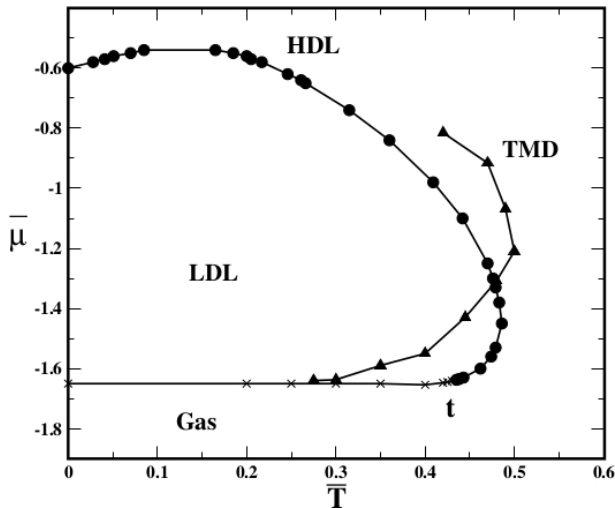
Simplest Model for Polymorphism? Bell Lattice

Szortyka, Fiore, Henriques, MCB, JCP 131, 164506 (2009)



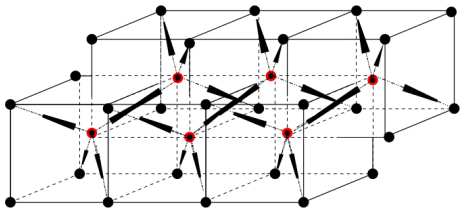
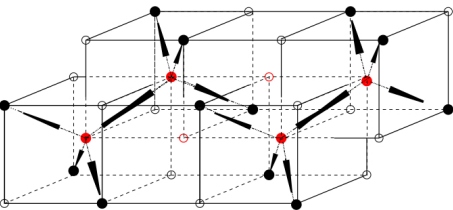
Simplest Model for Polymorphism? Bell Phase Diagram

Szortyka, Fiore, Henriques, MCB, JCP 131, 164506 (2009)



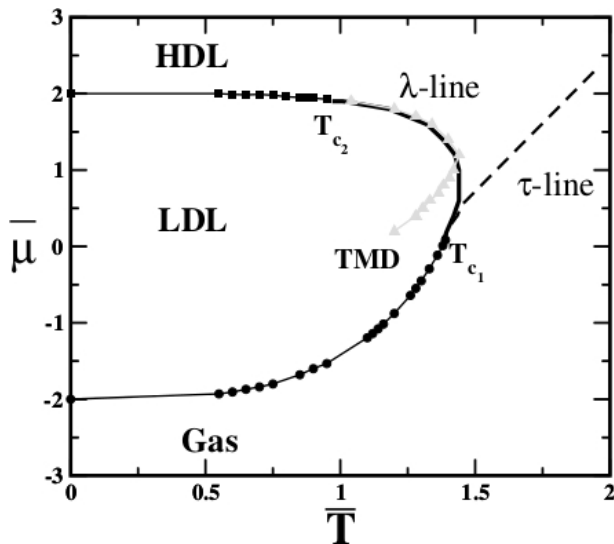
Simplest Model for Polymorphism? 3d ALG

Girardi, Szortyka, Henriques, MCB, JCP 132, 134904 (2010)



Simplest Model for Polymorphism? Bell Phase Diagram

Girardi, Szortyka, Henriques, MCB, JCP 132, 134904 (2010)



Summary

- ▶ Competition can lead to two liquid phases
- ▶ Competition can lead to density anomaly
- ▶ Are these two things connected?