

## Dipolmomente einiger Moleküle

TABLE 4.1 Dipole moments of molecules, bonds, and molecular groups (in Debye units:  $1 \text{ D} = 3.336 \times 10^{-30} \text{ C m}$ )<sup>a</sup>

<i>Molecules</i>			
Alkanes	0 <sup>b</sup>	H <sub>2</sub> O	1.85
C <sub>6</sub> H <sub>6</sub> (benzene)	0	CH <sub>3</sub> OH, C <sub>2</sub> H <sub>5</sub> OH	1.7
CCl <sub>4</sub>	0	Hexanol, octanol	1.7
CO <sub>2</sub>	0	C <sub>6</sub> H <sub>11</sub> OH (cyclohexanol)	1.7
CO	0.11	CH <sub>3</sub> COOH (acetic acid)	1.7
CHCl <sub>3</sub> (chloroform)	1.06	C <sub>2</sub> H <sub>4</sub> O (ethylene oxide)	1.9
HCl	1.08	CH <sub>3</sub> COCH <sub>3</sub> (acetone)	2.9
NH <sub>3</sub>	1.47	HCONH <sub>2</sub> (formamide)	3.7
SO <sub>2</sub>	1.62	C <sub>6</sub> H <sub>5</sub> OH (phenol)	1.5
CH <sub>3</sub> Cl	1.87	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub> (aniline)	1.5
NaCl	8.5	C <sub>6</sub> H <sub>5</sub> Cl (chlorobenzene)	1.8
CsCl	10.4	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub> (nitrobenzene)	4.2
<i>Bond moments</i>			
C—H <sup>+</sup>	0.4	C—C	0
N—H <sup>+</sup>	1.31	C=C	0
O—H <sup>+</sup>	1.51	C <sup>+</sup> —N	0.22
F—H <sup>+</sup>	1.94	C <sup>+</sup> —O	0.74
		C <sup>+</sup> —Cl	1.5–1.7
		N <sup>+</sup> —O	0.3
		C <sup>+</sup> =O	2.3–2.7
		N <sup>+</sup> =O	2.0
<i>Group moments</i>			
C— <sup>+</sup> OH	1.65	C— <sup>+</sup> CH <sub>3</sub>	0.4
C— <sup>+</sup> NH <sub>2</sub>	1.2–1.5	C <sup>+</sup> —NO <sub>2</sub>	3.1–3.8
		C— <sup>+</sup> COOH	1.7
		C— <sup>+</sup> OCH <sub>3</sub>	1.3

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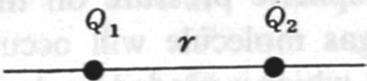
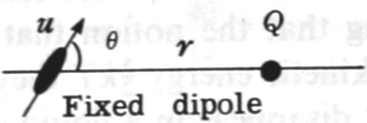
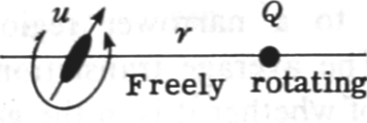
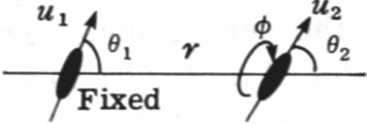
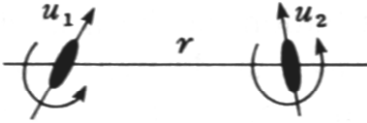
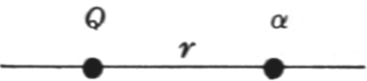
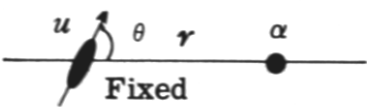
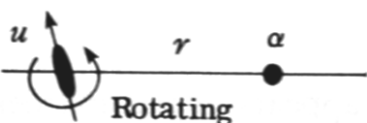
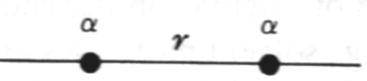
## Polarisierbarkeit einiger Moleküle

TABLE 5.1 Electronic polarizabilities  $\alpha_0$  of atoms, molecules, bonds, and molecular groups<sup>a</sup>

<i>Atoms and molecules</i>					
He	0.20	NH <sub>3</sub>	2.3	CH <sub>2</sub> =CH <sub>2</sub>	4.3
H <sub>2</sub>	0.81	CH <sub>4</sub>	2.6	C <sub>2</sub> H <sub>6</sub>	4.5
H <sub>2</sub> O	1.48	HCl	2.6	Cl <sub>2</sub>	4.6
O <sub>2</sub>	1.60	CO <sub>2</sub>	2.6	CHCl <sub>3</sub>	8.2
Ar	1.63	CH <sub>3</sub> OH	3.2	C <sub>6</sub> H <sub>6</sub>	10.3
CO	1.95	Xe	4.0	CCl <sub>4</sub>	10.5
<i>Bond polarizabilities</i>					
Aliphatic	C—C	0.48	C—O	0.60	
Aromatic	C $\cdots$ C	1.07	C=O	1.36	
	C=C	1.65	N—H	0.74	
Aliphatic	C—H	0.65	C—Cl	2.60	
	O—H	0.73	C—Br	3.75	
<i>Molecular groups</i>					
	C—O—H	1.28	CH <sub>2</sub>	1.84	
	C—O—C	1.13	Si—O—Si	1.39	
	C—NH <sub>2</sub>	2.03	Si—OH	1.60	

<sup>a</sup> Polarizabilities  $\alpha_0$  are given in units of  $(4\pi\epsilon_0)\text{\AA}^3 = (4\pi\epsilon_0)10^{-30} \text{ m}^3 = 1.11 \times 10^{-40} \text{ C}^2 \text{ m}^2 \text{ J}^{-1}$ . Note that when molecules are dissolved in a solvent medium their polarizability can change by up to 10%. Data compiled from Denbigh (1940), Hirschfelder *et al.* (1954) and Smyth (1955).

# Übersicht Wechselwirkungen

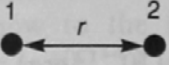
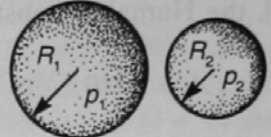
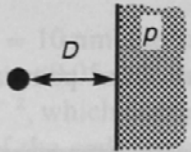
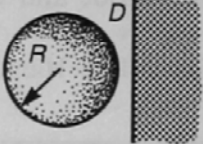
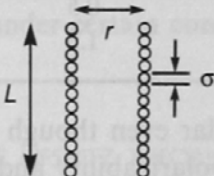
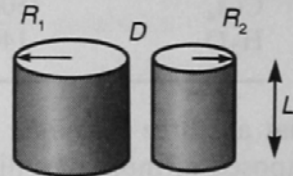
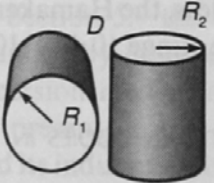
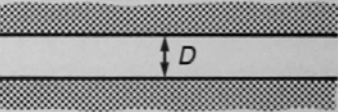
Charge-charge		$Q_1 Q_2 / 4\pi\epsilon_0 r$ (Coulomb energy)
Charge-dipole		$-Qu \cos \theta / 4\pi\epsilon_0 r^2$
		$-Q^2 u^2 / 6(4\pi\epsilon_0)^2 kTr^4$
Dipole-dipole		$-u_1 u_2 [2 \cos \theta_1 \cos \theta_2 - \sin \theta_1 \sin \theta_2 \cos \phi] / 4\pi\epsilon_0 r^3$
		$-u_1^2 u_2^2 / 3(4\pi\epsilon_0)^2 kTr^6$ (Keesom energy)
Charge-non-polar		$-Q^2 \alpha / 2(4\pi\epsilon_0)^2 r^4$
		$-u^2 \alpha (1 + 3 \cos^2 \theta) / 2(4\pi\epsilon_0)^2 r^6$
Dipole-non-dipolar		$-u^2 \alpha / (4\pi\epsilon_0)^2 r^6$ (Debye energy)
Two non-polar molecules		$\frac{3}{4} \frac{h\nu \alpha^2}{(4\pi\epsilon_0)^2 r^6}$ (London dispersion energy)

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## Relative Stärke der verschiedenen Van der Waals - Wechselwirkungen

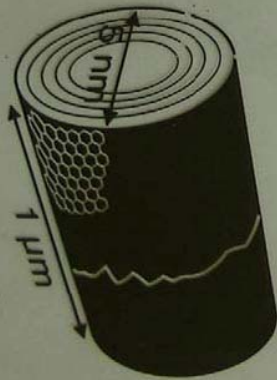
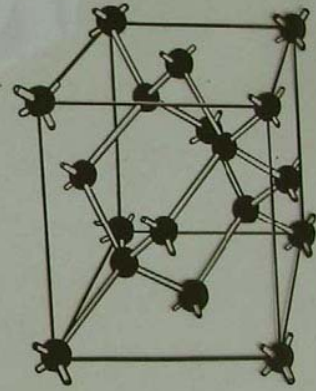
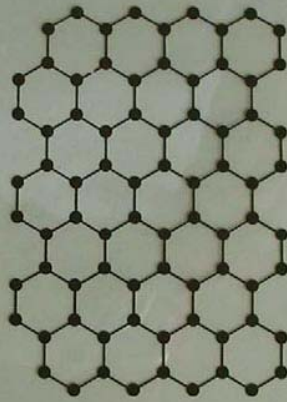
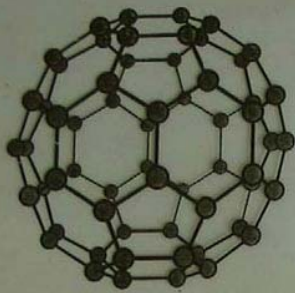
Interacting molecules	Electronic polarizability $\frac{\alpha_0}{4\pi\epsilon_0}$ ( $10^{-30} \text{ m}^3$ )	Permanent dipole moment $u$ (D) <sup>a</sup>	Ionization potential $I = h\nu_1$ (eV) <sup>b</sup>	Induktion (Debye)	Orientierung (Keesom)	Dispersion (London)
				$\frac{C_{\text{ind}}}{2u^2\alpha_0}$ $(4\pi\epsilon_0)^2$	$\frac{C_{\text{orient}}}{u^4/3kT}$ $(4\pi\epsilon_0)^2$	$\frac{C_{\text{disp}}}{3\alpha_0^2 h\nu_1}$ $4(4\pi\epsilon_0)^2$
Ne-Ne	0.39	0	21.6	0	4	4
CH <sub>4</sub> -CH <sub>4</sub>	2.60	0	12.6	0	0	102
HCl-HCl	2.63	1.08	12.7	6	11	106
HBr-HBr	3.61	0.78	11.6	4	3	182
HI-HI	5.44	0.38	10.4	2	0.2	370
CH <sub>3</sub> Cl-CH <sub>3</sub> Cl	4.56	1.87	11.3	32	101	282
NH <sub>3</sub> -NH <sub>3</sub>	2.26	1.47	10.2	10	38	63
H <sub>2</sub> O-H <sub>2</sub> O	1.48	1.85	12.6	10	96	33
Dissimilar molecules				$\frac{u_1^2\alpha_{02} + u_2^2\alpha_{01}}{(4\pi\epsilon_0)^2}$	$\frac{u_1^2u_2^2/3kT}{(4\pi\epsilon_0)^2}$	$\frac{3\alpha_{01}\alpha_{02}h\nu_1\nu_2}{2(4\pi\epsilon_0)^2(\nu_1 + \nu_2)}$
	Ne-CH <sub>4</sub>			0	0	19
	HCl-HI			7	1	197
	H <sub>2</sub> O-Ne			1	0	11
	H <sub>2</sub> O-CH <sub>4</sub>			9	0	58

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<p>Two atoms</p>  <p><math>w = -C/r^6</math></p>	<p>Two spheres</p>  <p><math>W = \frac{-A}{6D} \frac{R_1 R_2}{(R_1 + R_2)}</math></p>
<p>Atom-surface</p>  <p><math>w = -\pi C\rho/6D^3</math></p>	<p>Sphere-surface</p>  <p><math>W = -AR/6D</math></p>
<p>Two parallel chain molecules</p>  <p><math>W = -3\pi CL/8\sigma^2 r^5</math></p>	<p>Two cylinders</p>  <p><math>W = \frac{AL}{12\sqrt{2} D^{3/2}} \left( \frac{R_1 R_2}{R_1 + R_2} \right)^{1/2}</math></p>
<p>Two crossed cylinders</p>  <p><math>W = -A\sqrt{R_1 R_2}/6D</math></p>	<p>Two surfaces</p>  <p><math>W = -A/12\pi D^2</math> per unit area</p>

Wechselwirkungen zwischen verschiedenen ausgedehnten Objekten

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Forces



# Recognition

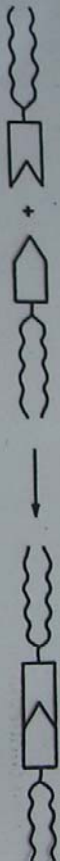
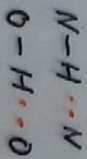
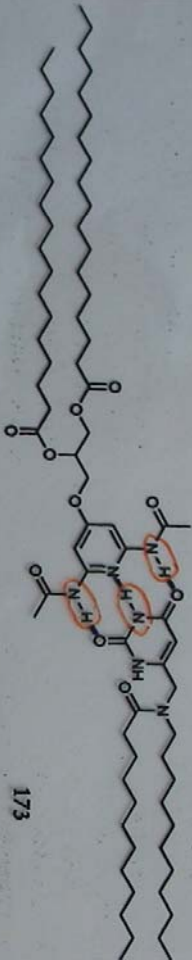


Fig. 38. Formation of a mesogenic supermolecule from two complementary components



173

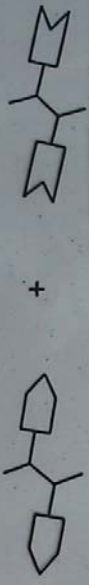
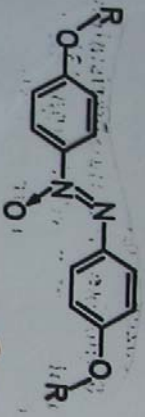


Fig. 39. Formation of a polymeric supramolecular species by association of two complementary ditopic components.

# Flüssig Kristalle



$R = CH_3$

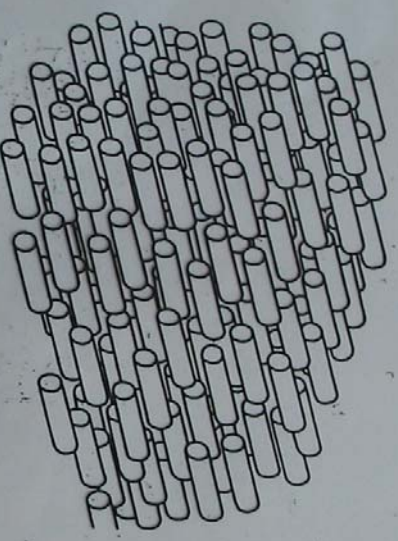


Abb. 19. Phasestruktur eines nematicen Flüssigkristalls

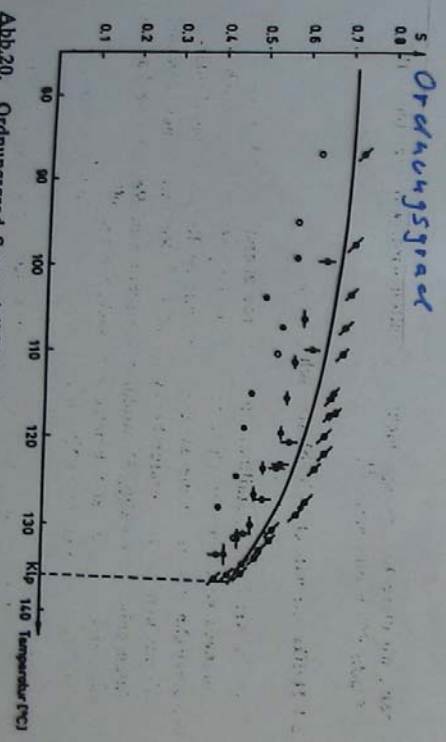


Abb. 20. Ordnungsgrad  $S$  von 4,4'-Dimethoxyazobenzene (2a), bestimmt aus:  $\bullet$  = IR-Spektren,  $\circ$  = UV-Spektren,  $\phi$  = diamagn. Suszeptibilität,  $\ominus$  = Brechungsindex bei 546 nm,  $\otimes$  = Protonenresonanz. Die ausgezogene Kurve wurde nach der Theorie berechnet (42)

Chemisorption

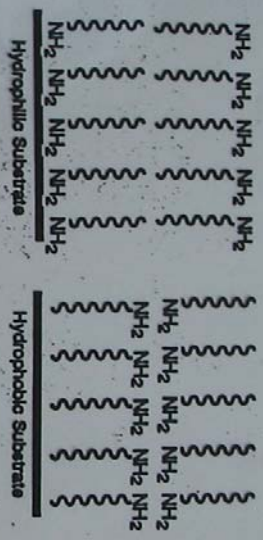


Figure 142. A tail-to-tail bilayer (left) and a head-to-head bilayer (right) of ODA.

Surfactant

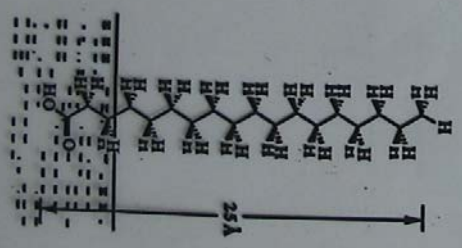
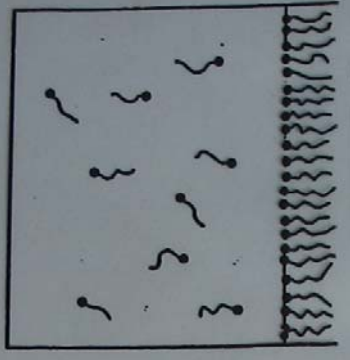


Figure 2.5. A stearic acid molecule on the water-air interface.

gold-colloid

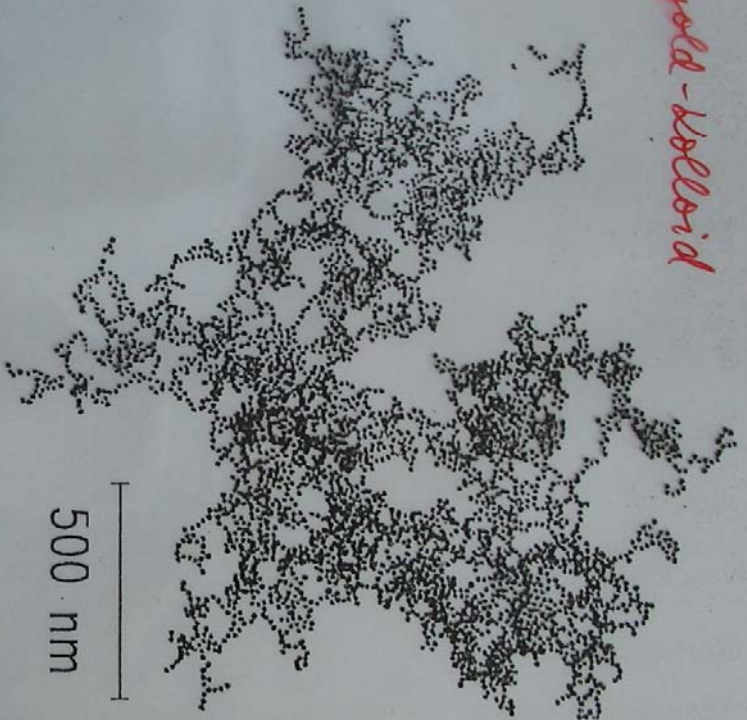


Fig. 7. The transmission electron microscope image of a gold colloidal aggregate (Weitz and Oliveria<sup>21</sup>).

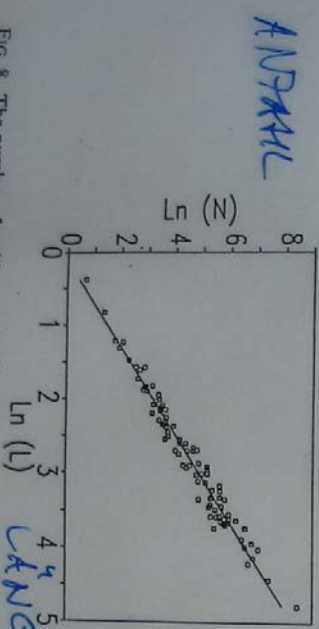


Fig. 8. The number of gold particles  $N$  plotted versus the length scale  $L$  of the colloidal aggregate in Fig. 1. The slope of the log-log plot gives the fractal dimension  $d = 1.75$ . The unit of  $L$  is 14.5 nm (Weitz and Oliveria<sup>21</sup>).



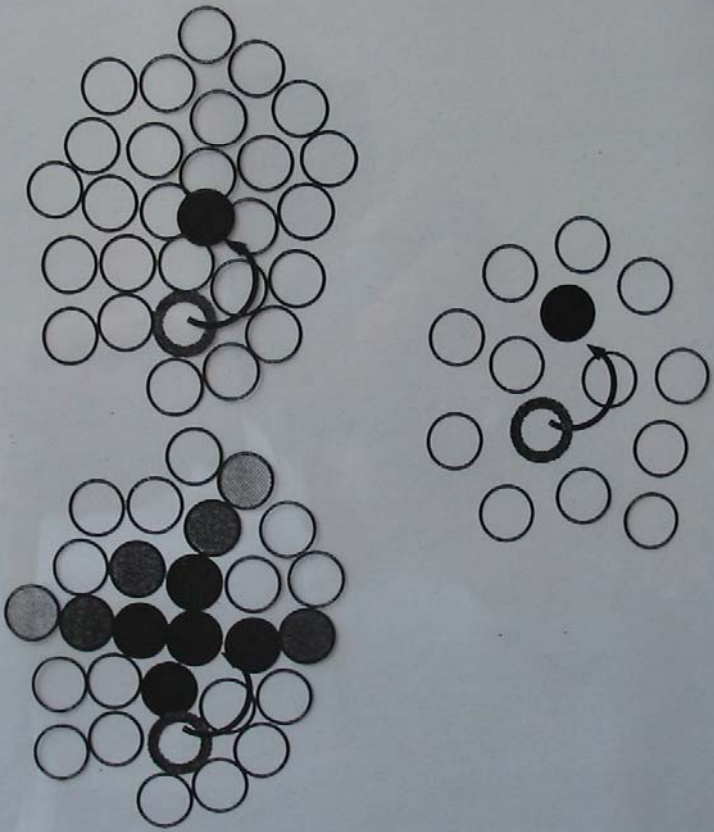


Fig. 2.13 The idea of cooperativity in diffusive motion of a molecule in a glass-forming liquid. At high temperatures and low densities (top) a molecule is able to jump to a new position without the necessity for wholesale rearrangement of its neighbours. At lower temperatures and higher densities (bottom), in order for one molecule to be able to make a move (left), some of its neighbours (shown shaded) must move cooperatively to make room (right).

The theory of gelation

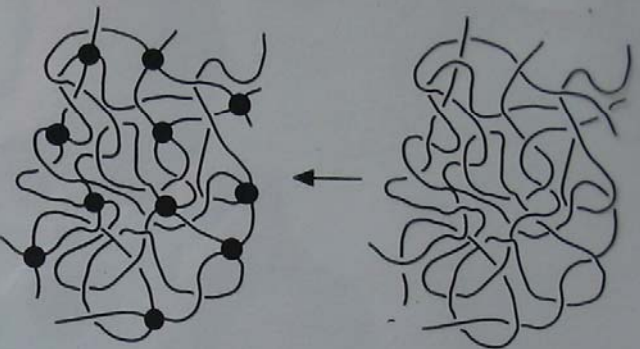


Fig. 6.2 Schematic of a vulcanisation reaction. The system consists of a mixture of long chains. Initially, the chains are entangled but not covalently linked. The reaction proceeds by chemically linking adjacent chains, leading to the formation of an infinite network.

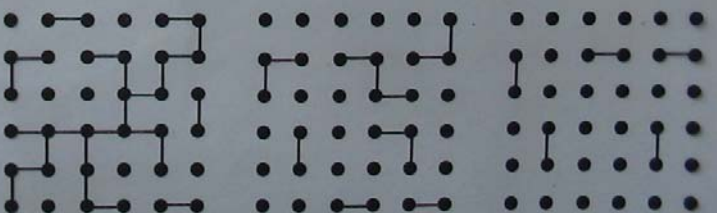
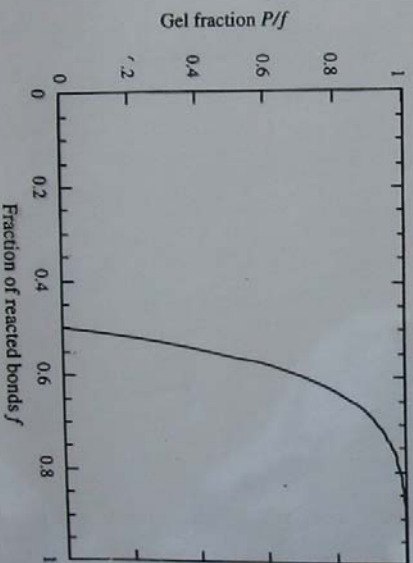


Fig. 6.6 The percolation model. We start with array of points, to which bonds are added at random (top). As more bonds are added, clusters of points are formed (middle), which ultimately join to form a cluster which spans the entire system (bottom).



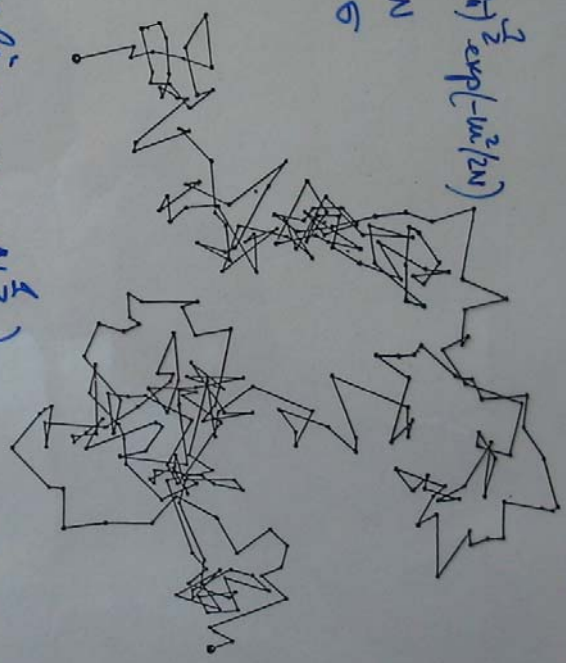
2+1D DDH Walk (Brownian Bewegung)

$$P(w, N) = (R^2)^{\frac{3}{2}} \cdot \exp(-w^2/2N)$$

$$N \rightarrow 4N$$

$$26 \rightarrow 26$$

$$D=2$$



(Nettoweglänge  $\approx N^{\frac{1}{2}}$ )

