Two Pieces of the Simulation Work:
Study of Electronic Structures of Organic Molecules and Correlation between Microstructures and Elastic Response of Organogel Networks

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CONTENTS

- Basic information
- Research work

Part 1: 2005-09.2006 in Shandong University, China

study of electronic structures of organic molecules through

Quantum Chemical Software Gaussian 98.

Part 2: 09.2006-10.2007 in National University of Singapore, Singapore

investigate the correlation between microstructures and elastic response of planar spherulitic networks.

- Recent condition

BASIC INFORMATION

Name: Jinghua Shi

From: Anhui Province, China

2000-2004 B.S.

Shandong University,

Shandong, China

Majoring in Applied Physics

2004-2007 M. E.

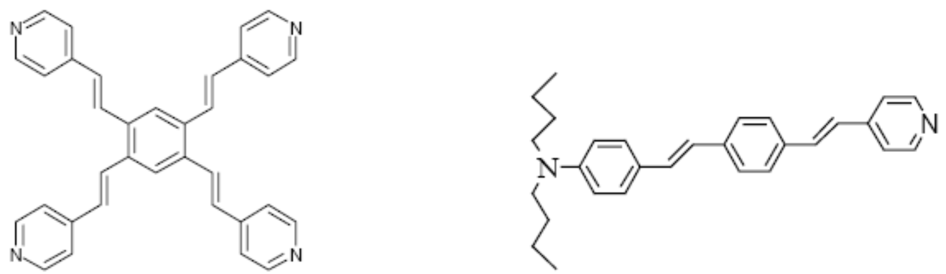
Shandong University,

Majoring in Material Physics and Chemistry

RESEARCH WORK: part 1

Research group of Prof. Tao: Organic light emitting materials.

For example:



TKPVB **DBASVP**

Scheme 1 molecule structure of TKPVB and DBASVP

Applications: light emitting diodes (LEDs), organic lasers, photovoltaic cells, etc.

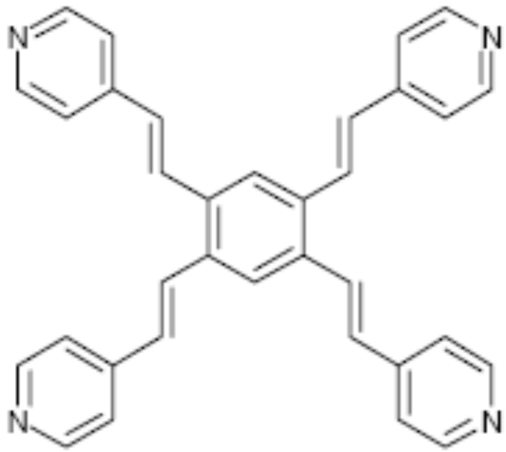
My task:

Simulation of the organic molecules and materials;

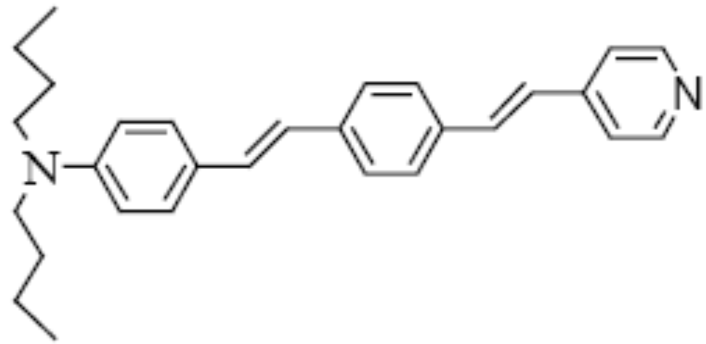
Calculation their electronic structure

→ Aim to understand the physical mechanism of experimental phenomenon

Example: J. Phys. Chem. B 2006, 110, 19711-19716



TKPVB



DBASVP

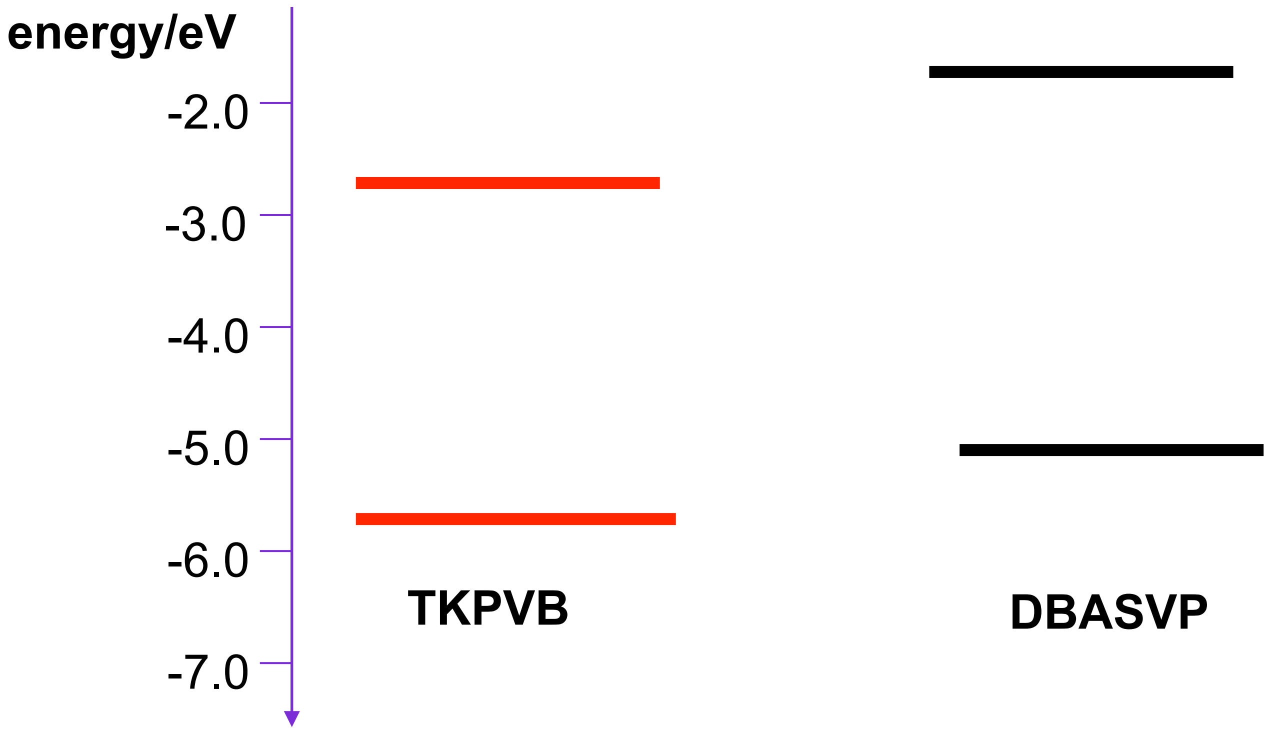
Scheme 1 molecule structure of TKPVB and DBASVP

Geometries of the two molecules are both optimized at density hybrid functional level (b3lyp/6-31g) using Gaussian98 package

RESULTS

TKPVB: the energy of **HOMO** is -5.96eV,
LUMO is -2.67eV

DBASVP: the energy of **HOMO** is -5.17eV,
LUMO is -2.01eV



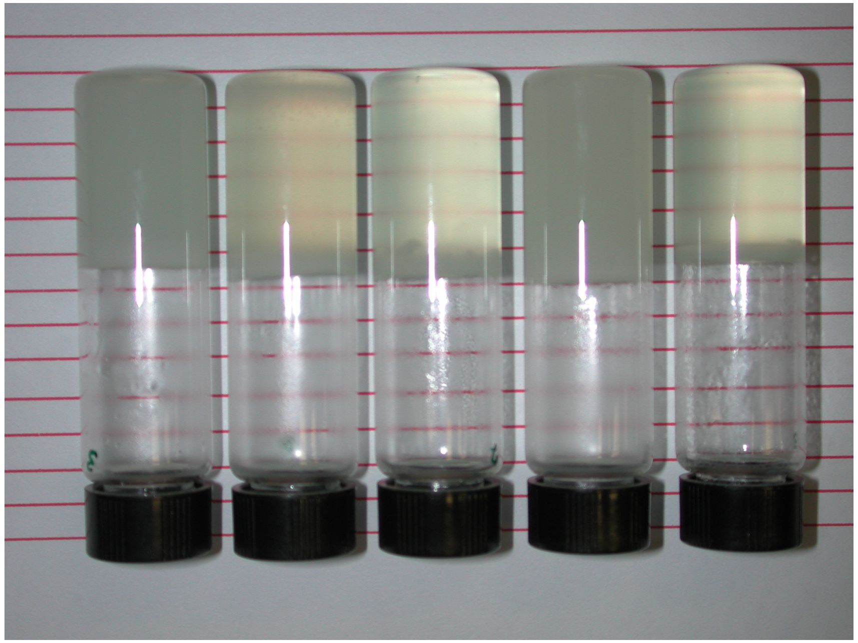
TKPVB: electron distribution of HOMO and LUMO

DBASVP: electron distribution of HOMO and LUMO

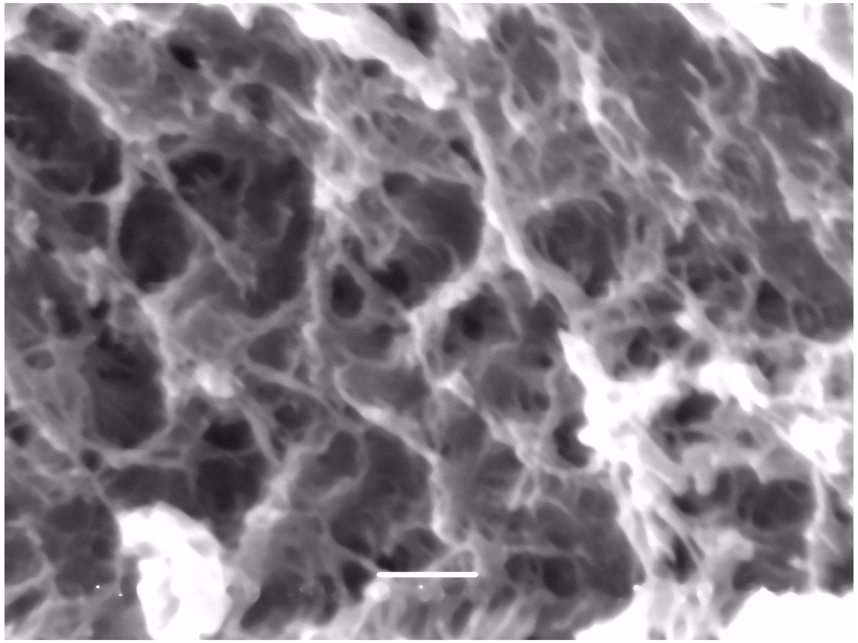
RESEARCH WORK: part 2

Research group of Prof. Liu:

Small-molecule-mass organogels (SMOGs):some low-mass molecules can gel organic solvent at very low concentration (<2 wt%) to form organogel.

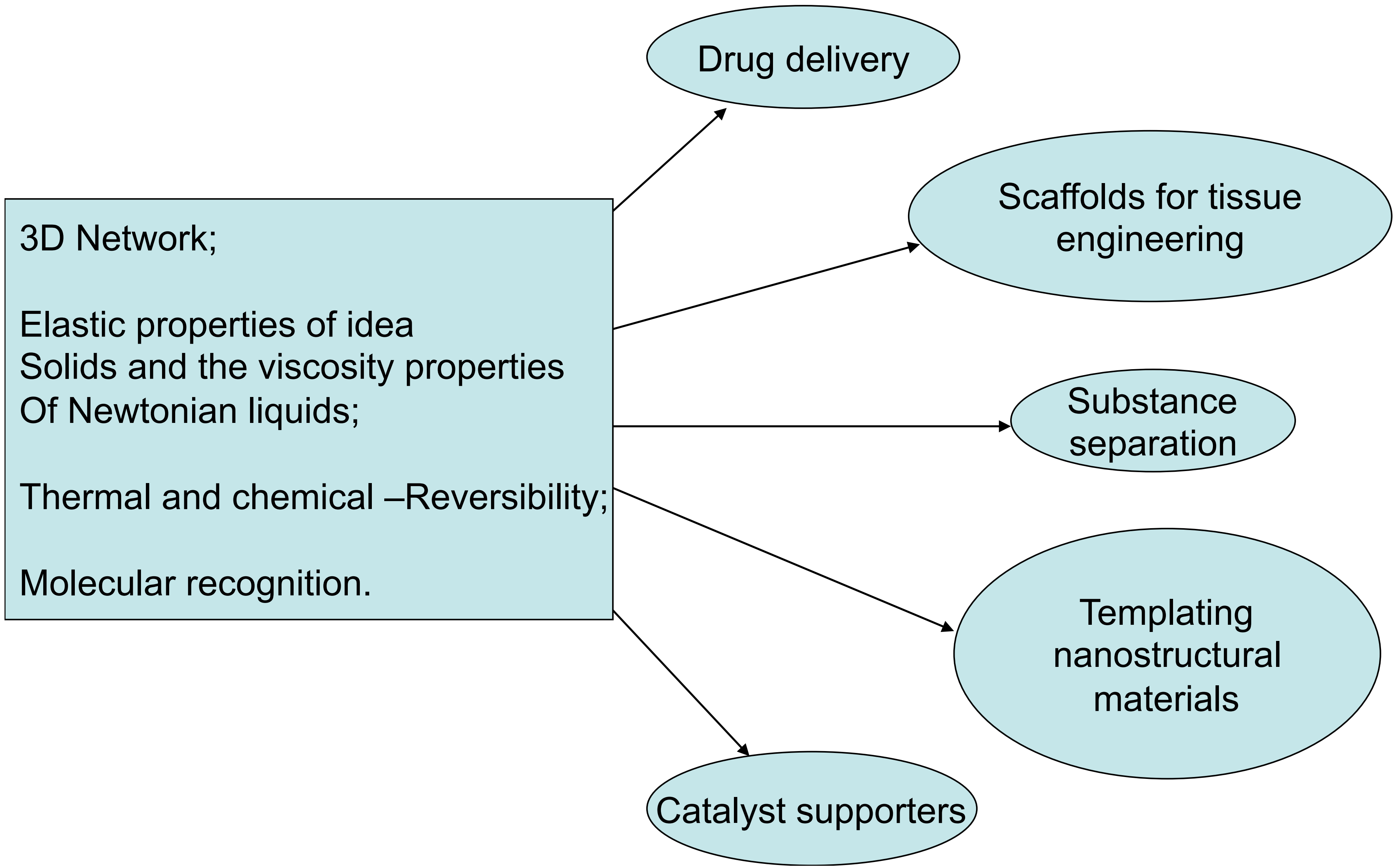


Consisting of 3D interconnected fiber networks trapping organic liquid.



Optical micrograph of an organogel network

PROPERTIES AND APPLICATIONS



My task:

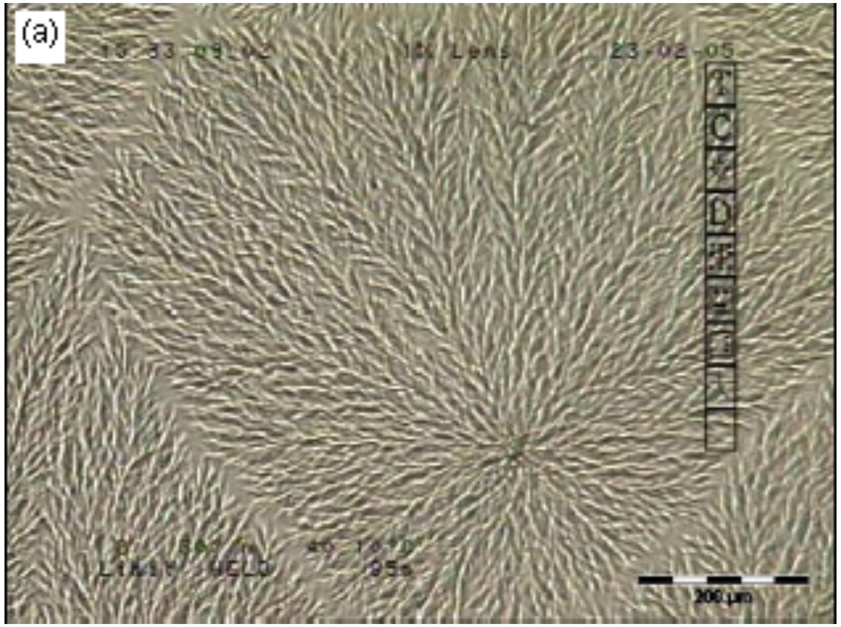
investigate the relationship between microstructure of SMOGs and their macroscopic properties.

Aim to:

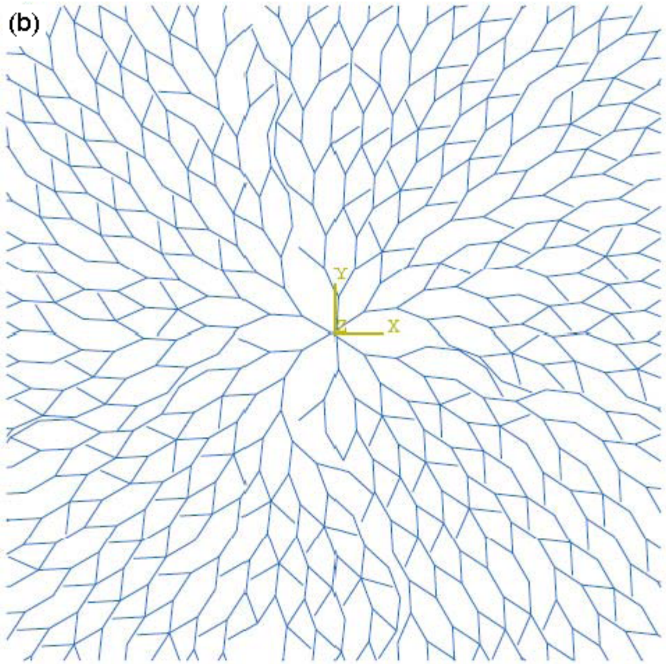
develop a new idea to design the SMOGs.

FIRST STEP WORK

A finite element method based on ABAQUS



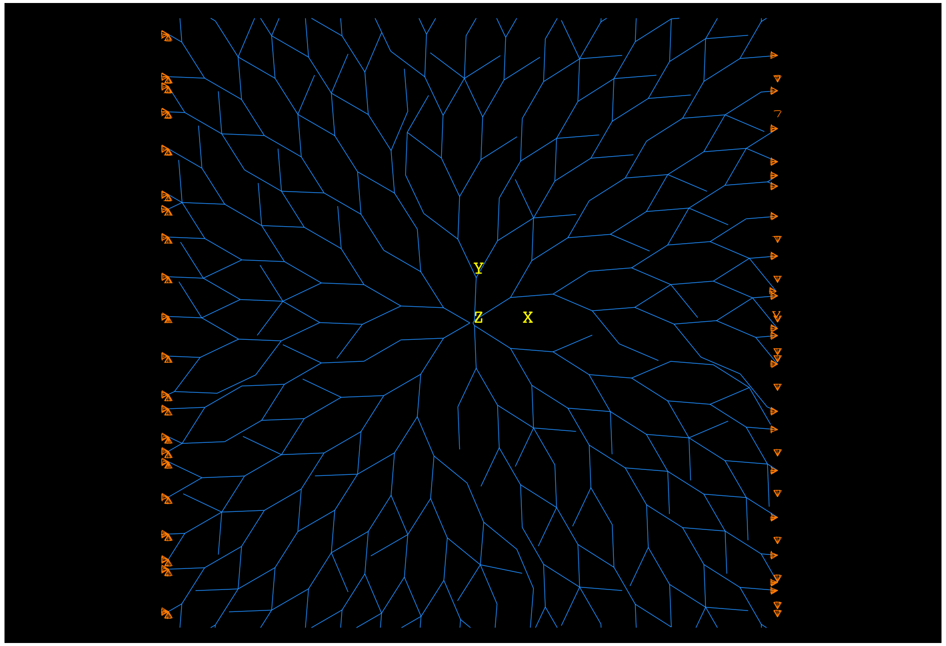
Optical micrograph of an organogel network



Simulation model: planar radial-growth network

Definition of elastic modulus of the network

$$E_{strain} = \frac{1}{2} G \times \gamma^2 \times L_x \times L_y \times 2r$$

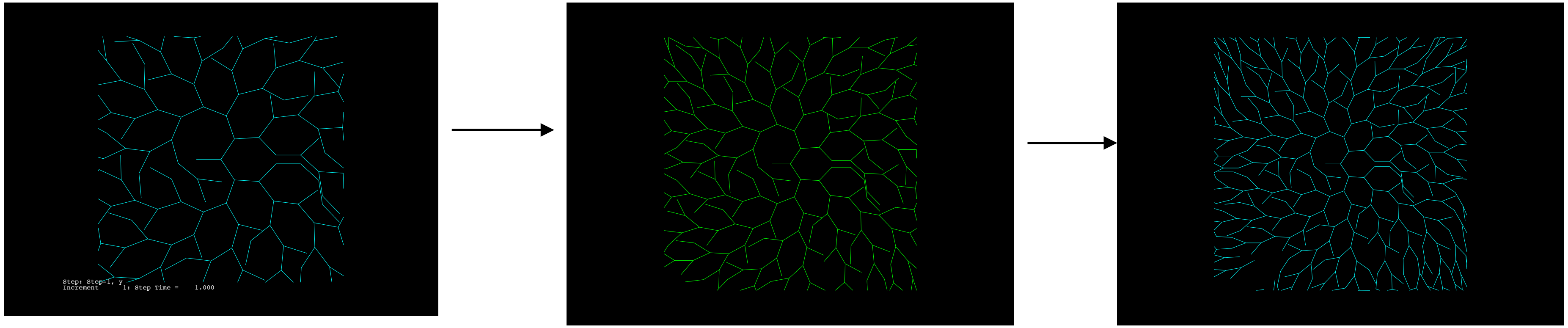


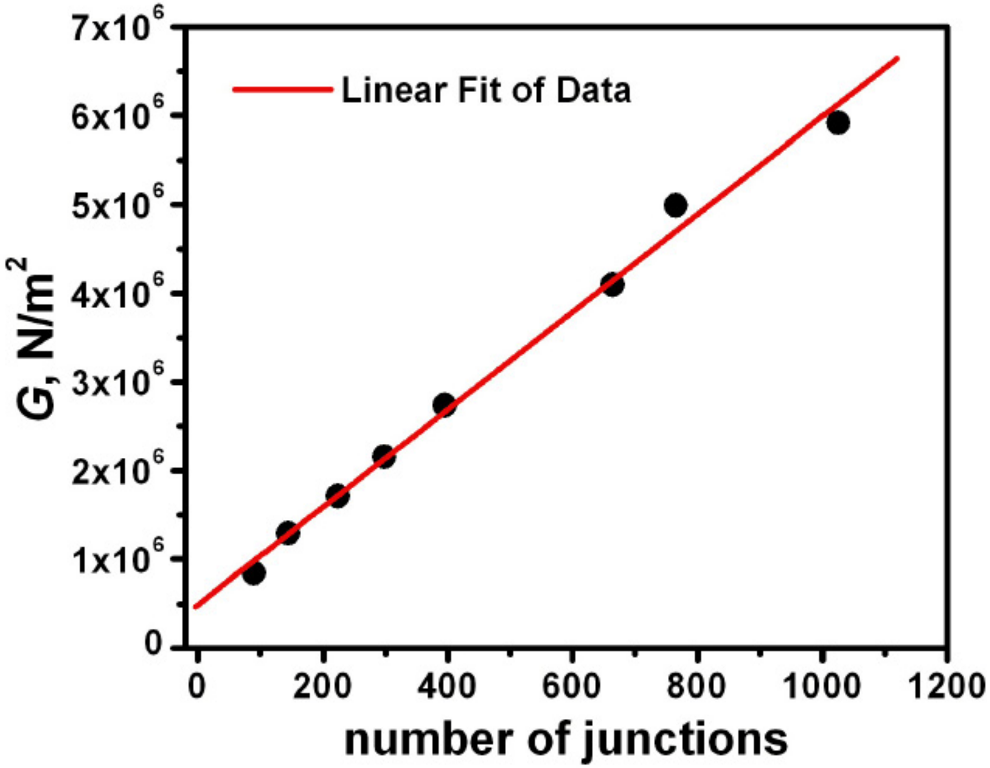
E_{strain}: strain energy;

G : shear modulus of the network; *γ*: the applied shear strain;

Lx、*Ly*: the length and width of the area;

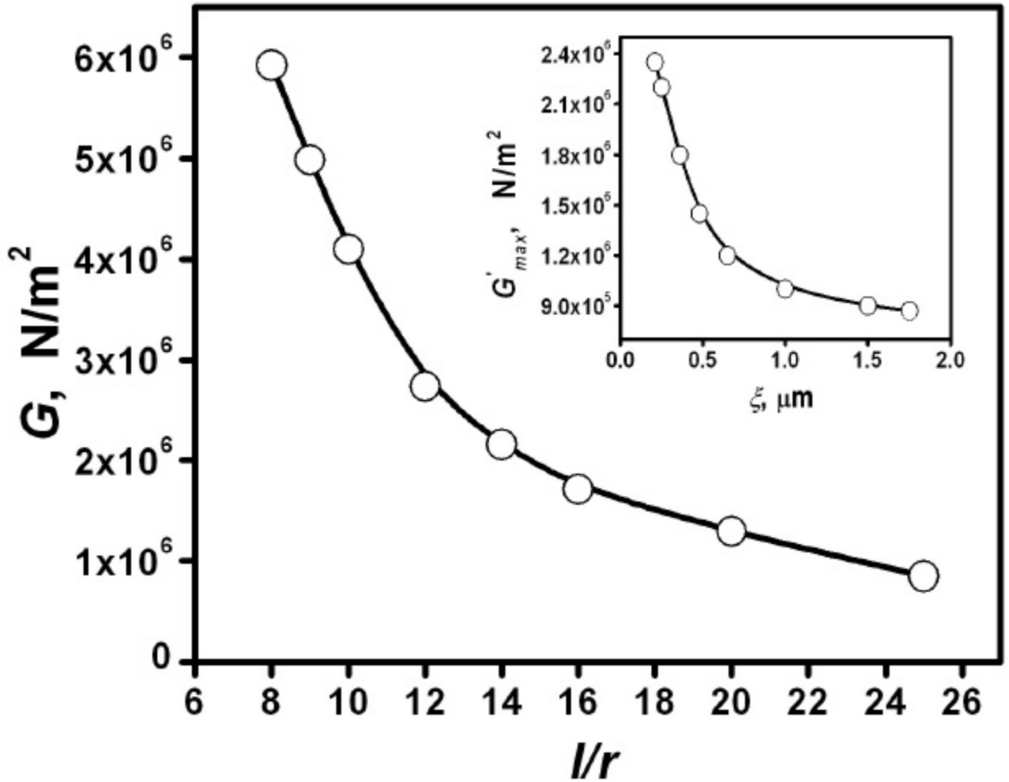
r: the radius of the fiber cross-section.





Effect of the junction density on *G*. Black circles are the simulation data, and the red line is to guide the eye.

***G* increases monotonically with the junction density.**

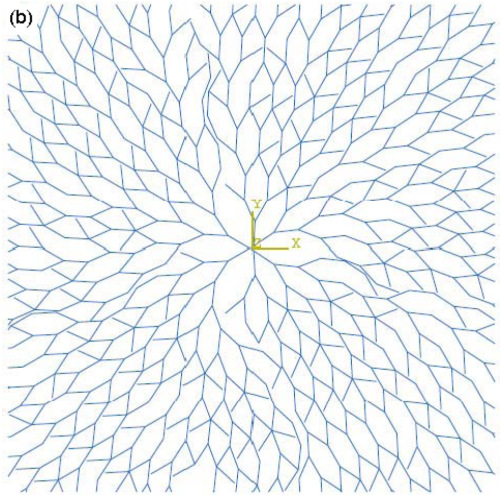


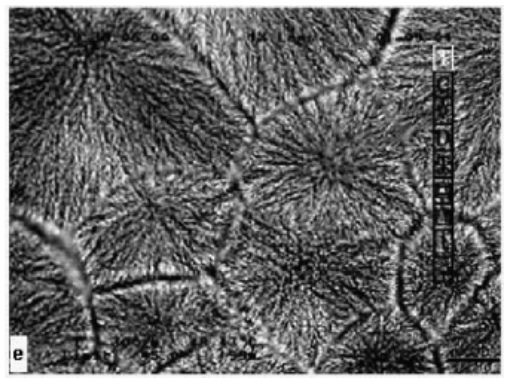
Effect of the fiber length *l* on G., where *r* is fixed. The inset is the experimental relationship between *G* and *ξ* (*ξ* is the correlation length, defined as the distance between two adjacent branching points along one fiber, and is proportional to *l* in the simulations).

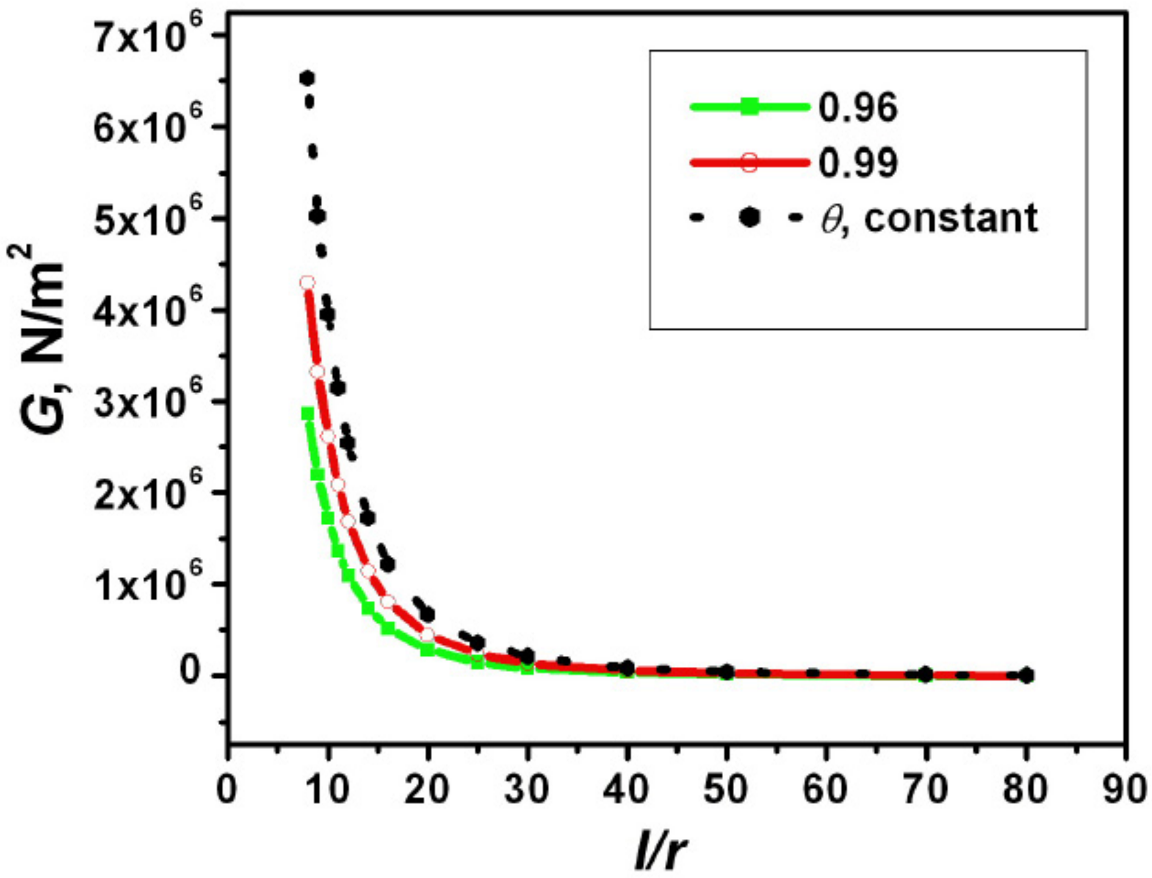
Simulation: $G \sim l^{-1.71}$。

Experiment：$G \sim \xi^{-0.49}$。

In another study (*J. Phys. Chem. B* 2007, 111, 5558), it gives rise to $G \sim \xi^{-1.5}$



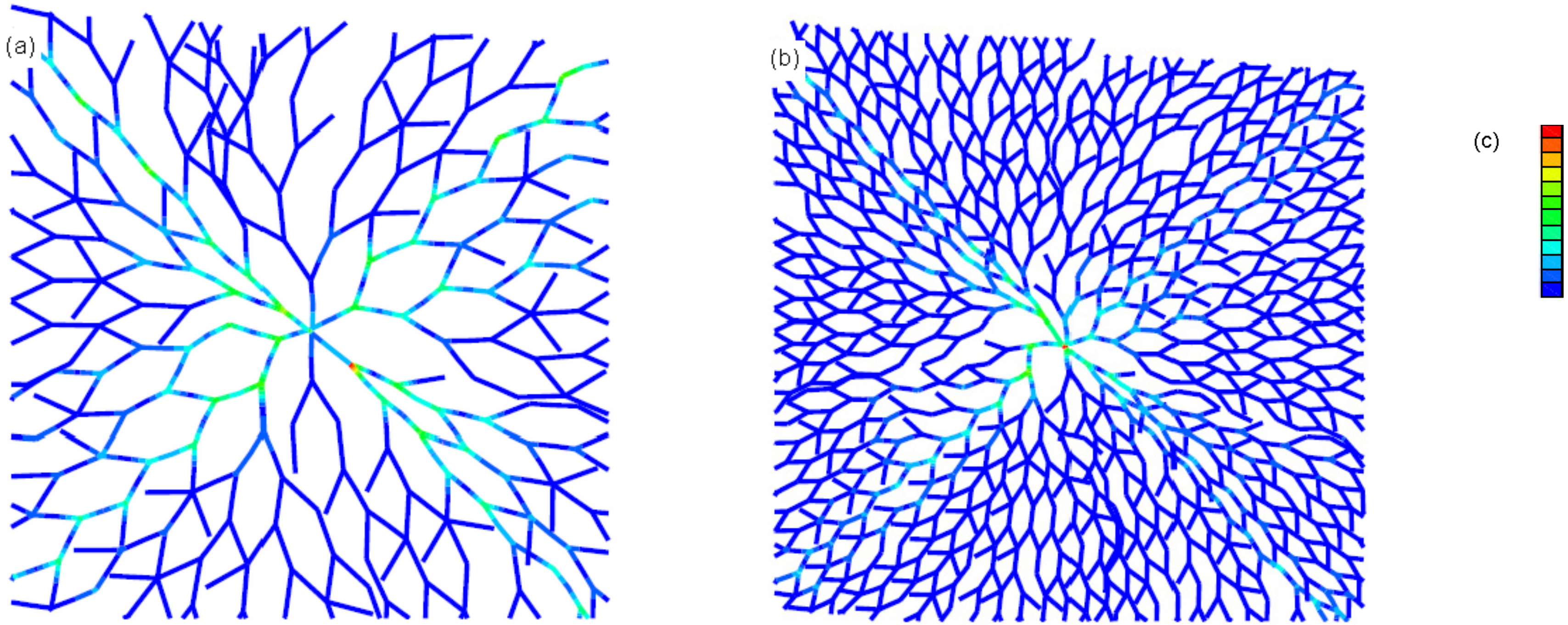




G' vs l/r where r is varied and l if fixed.

***l/r*<20: *G* increases drastically with *r*；**

***l/r*>20：the relation tends to level off.**



(a) Stress distribution in networks with a fiber aspect ratio of 16; (b) stress distribution in networks with a fiber aspect ration of 8; (c) stress distribution sequence: from red to blue the stress varies correspondingly from maximum to minimum.

The research results are published in J. Phys. Chem. B 2009, 113, 4549-4554.

RECENT CONDITON

2008: get married and have a baby

2010 with my husband moved to Hamburg. During this time I learn German.

Thanks for your attention!