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Evaluation of Commercial Opportunities Within a Scientific Area

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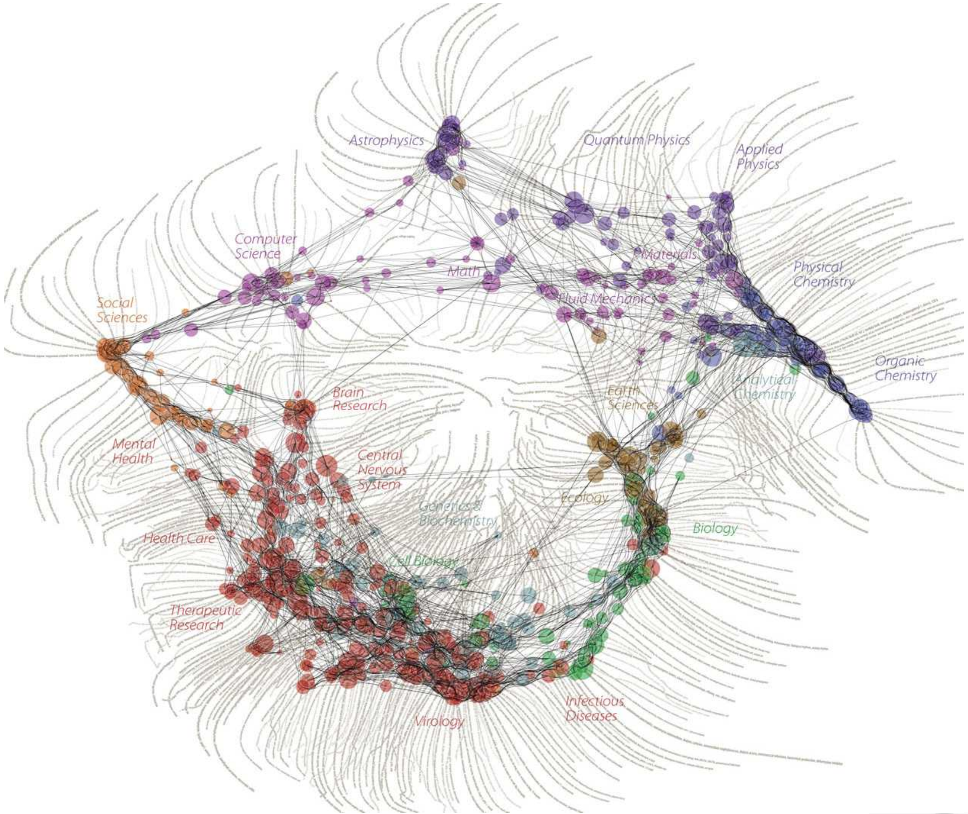

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Outline

- Objectives and background
- Stories of what we’ve tried, what has worked and what hasn’t
- Wrap-up with lessons learned

Objectives

- Published objectives
  - Experience state-of-the-art methods for visualization of science and technology
  - Understand how a map of the scientific terrain anticipates where technical/commercial opportunities are likely to arise
  - Analyze commercial opportunities from the emerging field of nanotechnology

List of questions

- What does the field look like?
- What are the key topics? What are the hot topics?
- Where are things likely to go in the future?
- Who are the key players? Who should I be worried about? Who should I collaborate with? (people and institutions)
- Is there commercial opportunity?
- What are my competitors doing? Are they any good?
- What is country X doing in field Y?
- My technology needs a tweak. Is there science that would inform this? If so, where?

I've been asked a question, now what?

Is my niche in bionanotechnology likely to produce commercial results?

- ➢ Get the right data
- ➢ Classify / categorize the data
- ➢ Analyze the data
- ➢ Report my results

Stumbling blocks

- Defining the field properly – getting the right data

11th International Conference on Scientometrics and Informetrics
Madrid, 25-27 June
[http://issi2007.cindoc.csic.es/]
Extended deadline for short papers or presentations: April 3
Call for papers and presentations
Workshop on:
Taking CiteSpace to Science: new applications to visualization programming

The visualization freeware CiteSpace was developed by Chaomei Chen at Drexel University, US. Originally it was meant as an instrument for analyzing paradigmatic shifts in scientific specialties. In several articles Chen has shown the abilities of the program, but **one of the weaknesses is the definition of a scientific field. We invite papers that discuss different approaches to this important problem.** How reliable are strategies on the basis of keywords, on subject codes, or on selected sets of journals? If researchers normally are active in many different journals covering 15-20 different subject codes what does that say about using the ISI codes for definition of specialties?

- Unclear understanding of how things evolve

Some things we've tried

- Look at the key journals
- Do keyword searches – big hairy boolean query
- Map all of science

Journal-based field definition

- Get papers from a list of journals
- Cluster, count, trend analysis, etc.
- But
  - Misses essential materials
  - Includes much outside topic area of interest

Keyword-based field definition

- Get individual papers
- Cluster, count, trend analysis, etc.
- Better field definition than journals; can be very good, but depends on exact query
- But
  - Usually requires many iterations with subject matter experts (SME) to refine the keyword list
  - Time-consuming
  - Misses essential material due to non-standard vocabulary

Mapping all of science

- Generate a map of science once, and use it over and over again
  - Initial work is time consuming
- Have SME supply seed information (papers)
  - Papers map to clusters and sets of terms
  - Give SME term lists of initial clusters and linked clusters and have them rate the term lists
  - Iterate 2-3 times, about an hour of SME time
- Better field definition than keywords
  - Very good focus on topics of interest due to iterative nature
  - Includes material that would not be found from keyword searches
  - Clearly shows linkages to other topics/fields
  - Current (topics) vs. reference (paradigm) distinction important – can't be shown using other methods

Example 1

What does the field of nanotechnology look like?

- Journal-based field definition

List of journals

- 10 core journals with NANO in the title
  - *Current Nanoscience*
  - *Fullerene Nanotubes and Carbon Nanostructures*
  - *IEEE Transactions on Nanotechnology*
  - *IEEE Transactions on Nanobioscience*
  - *Journal of Computational and Theoretical Nanoscience*
  - *Journal of Nanoparticle Research*
  - *Journal of Nanoscience and Nanotechnology*
  - *Nano Letters*
  - *Nanotechnology*
  - *Physica E: Low Dimensional Systems & Nanostructures*

- 2005: 2310 papers in these 10 journals

BUT …

- … if you do a boolean search on TAK (title, abstract, kwd)
  - Standard nano search string [self-assembl*, atomic force microsc*, scanning tunneling microsc*, molecular device, molecular motor, molecular sensor, molecular simulation, quantum comput*, quantum dot, quantum wire, nano* (omitting nanosecond, nanoliter, nanometer)]
- 2005: 56,000 papers in 2,600 journals
- Where are the nano- papers?

All over the place

rank	jnl	# nano papers	fraction	field
1	PHYS REV B	1818	27.0%	PHYS
2	APPL PHYS LETT	1583	34.5%	PHYS
3	J PHYS CHEM B	1456	41.5%	CHEM
4	P SOC PHOTO-OPT INS	1428	8.6%	OPT
5	LANGMUIR	998	53.5%	CHEM
6	J APPL PHYS	918	27.1%	PHYS
7	J AM CHEM SOC	788	22.5%	CHEM
8	PHYS REV LETT	687	17.9%	PHYS
9	MATER RES SOC SYMP P	682	36.8%	MATLS
10	NANOTECHNOLOGY	623	95.1%	NANO
11	CHEM MATER	519	48.9%	CHEM
12	AIP CONF PROC	503	9.5%	CHEM
13	THIN SOLID FILMS	502	34.7%	MATLS
14	NANO LETT	455	96.2%	NANO
15	POLYMER	441	32.0%	CHEM
16	JPN J APPL PHYS 1	431	21.8%	PHYS
17	APPL SURF SCI	421	36.0%	MATLS
18	J CHEM PHYS	409	14.3%	PHYS
19	ADV MATER	404	66.7%	MATLS
20	MACROMOLECULES	402	25.5%	CHEM
21	CHEM COMMUN	398	24.1%	CHEM
22	J CRYST GROWTH	396	31.9%	MATLS
23	MATER LETT	381	39.0%	MATLS
24	J MAGN MAGN MATER	364	29.6%	MATLS
25	CHEM PHYS LETT	355	23.0%	PHYS
26	SURF SCI	335	44.7%	MATLS
27	ANGEW CHEM INT EDIT	326	21.6%	CHEM
28	MATER SCI FORUM	310	11.6%	MATLS
29	CARBON	307	60.8%	CHEM
30	PHYSICA E	307	71.1%	NANO
33	J NANOSCI NANOTECHNO	302	91.2%	NANO
124	J NANOPART RES	87	100.0%	NANO
125	IEEE T NANOTECHNOL	86	75.4%	NANO
154	FULLER NANOTUB CAR N	72	71.3%	NANO
219	J COMPUT THEOR NANOS	46	76.7%	NANO
367	CURR NANOSCI	23	92.0%	NANO
434	IEEE T NANOBIOSCI	18	45.0%	NANO

Example 2

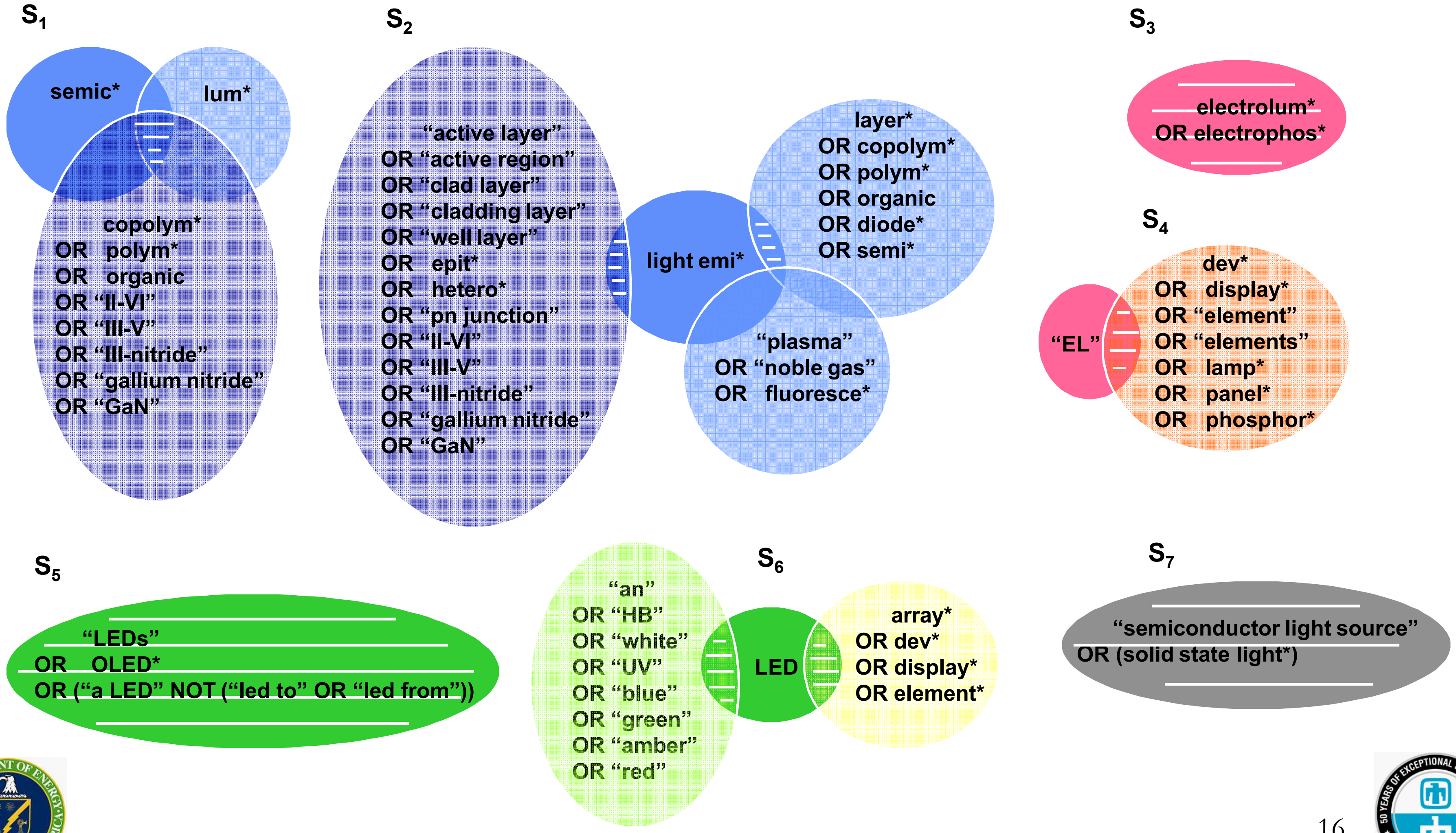
What are the hot current topics in the field of solid-state lighting (SSL)?

- Keyword-based field definition

SSL analysis, joint with Jeff Tsao, Sandia

Boolean search

$SSL = S_1 \text{ OR } S_2 \text{ OR } S_3 \text{ OR } S_4 \text{ OR } S_5 \text{ OR } S_6 \text{ OR } S_7$



S_1

semic*

lum*

copolym*
OR polym*
OR organic
OR "II-VI"
OR "III-V"
OR "III-nitride"
OR "gallium nitride"
OR "GaN"

S_2

"active layer"
OR "active region"
OR "clad layer"
OR "cladding layer"
OR "well layer"
OR epit*
OR hetero*
OR "pn junction"
OR "II-VI"
OR "III-V"
OR "III-nitride"
OR "gallium nitride"
OR "GaN"

light emi*

layer*
OR copolym*
OR polym*
OR organic
OR diode*
OR semi*

"plasma"
OR "noble gas"
OR fluoresce*

S_3

electrolum*
OR electrophos*

S_4

"EL"

dev*
OR display*
OR "element"
OR "elements"
OR lamp*
OR panel*
OR phosphor*

S_5

"LEDs"
OR OLED*
OR ("a LED" NOT ("led to" OR "led from"))

S_6

"an"
OR "HB"
OR "white"
OR "UV"
OR "blue"
OR "green"
OR "amber"
OR "red"

LED

array*
OR dev*
OR display*
OR element*

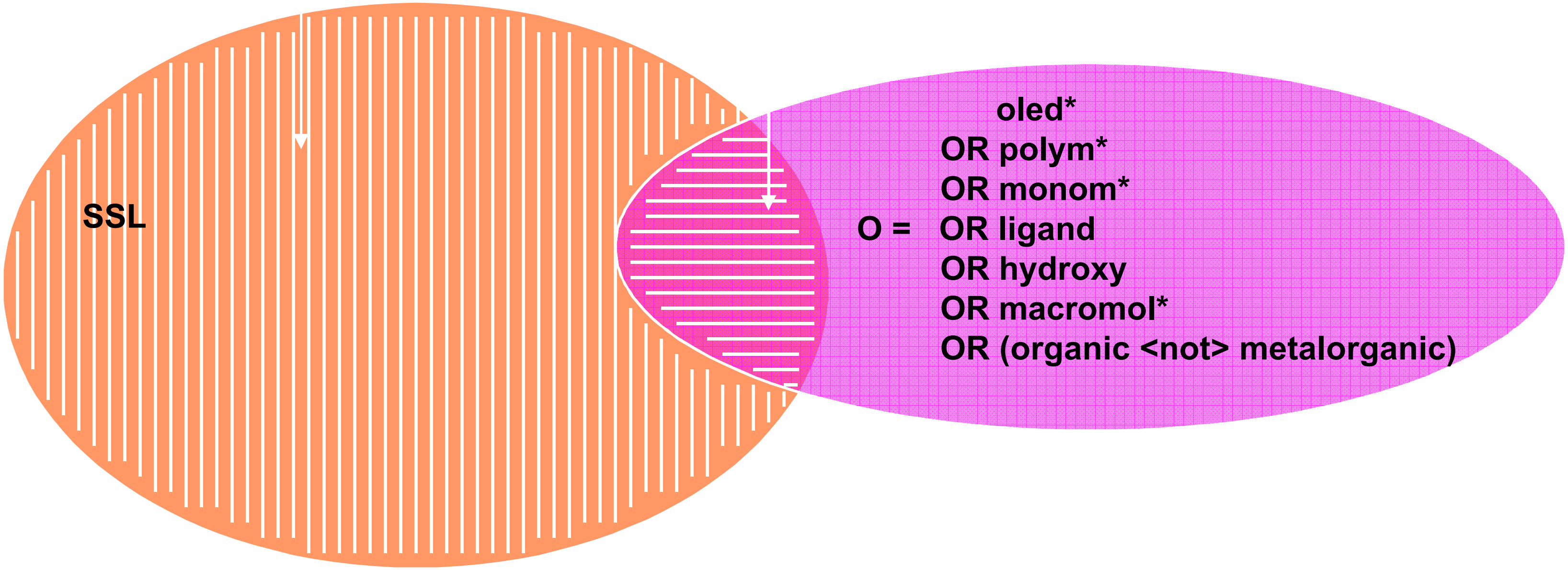
S_7

"semiconductor light source"
OR (solid state light*)

Partitioning the data

$SSL_{Inorganic}$ = SSL NOT Organic

$SSL_{Organic}$ = SSL AND Organic

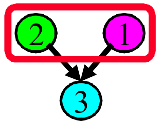


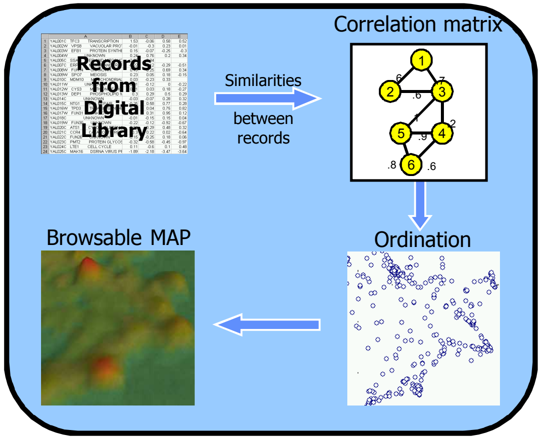
SSL

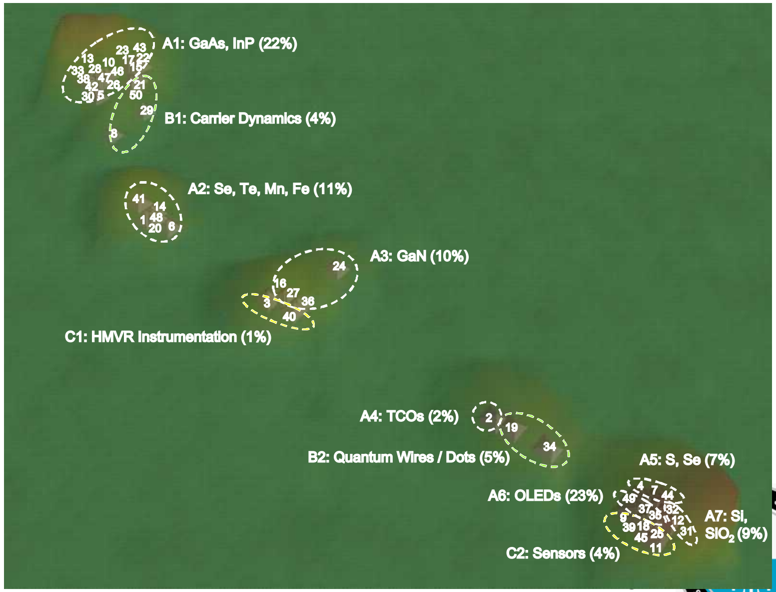
O = oled*
OR polym*
OR monom*
OR ligand
OR hydroxy
OR macromol*
OR (organic <not> metalorganic)

Process

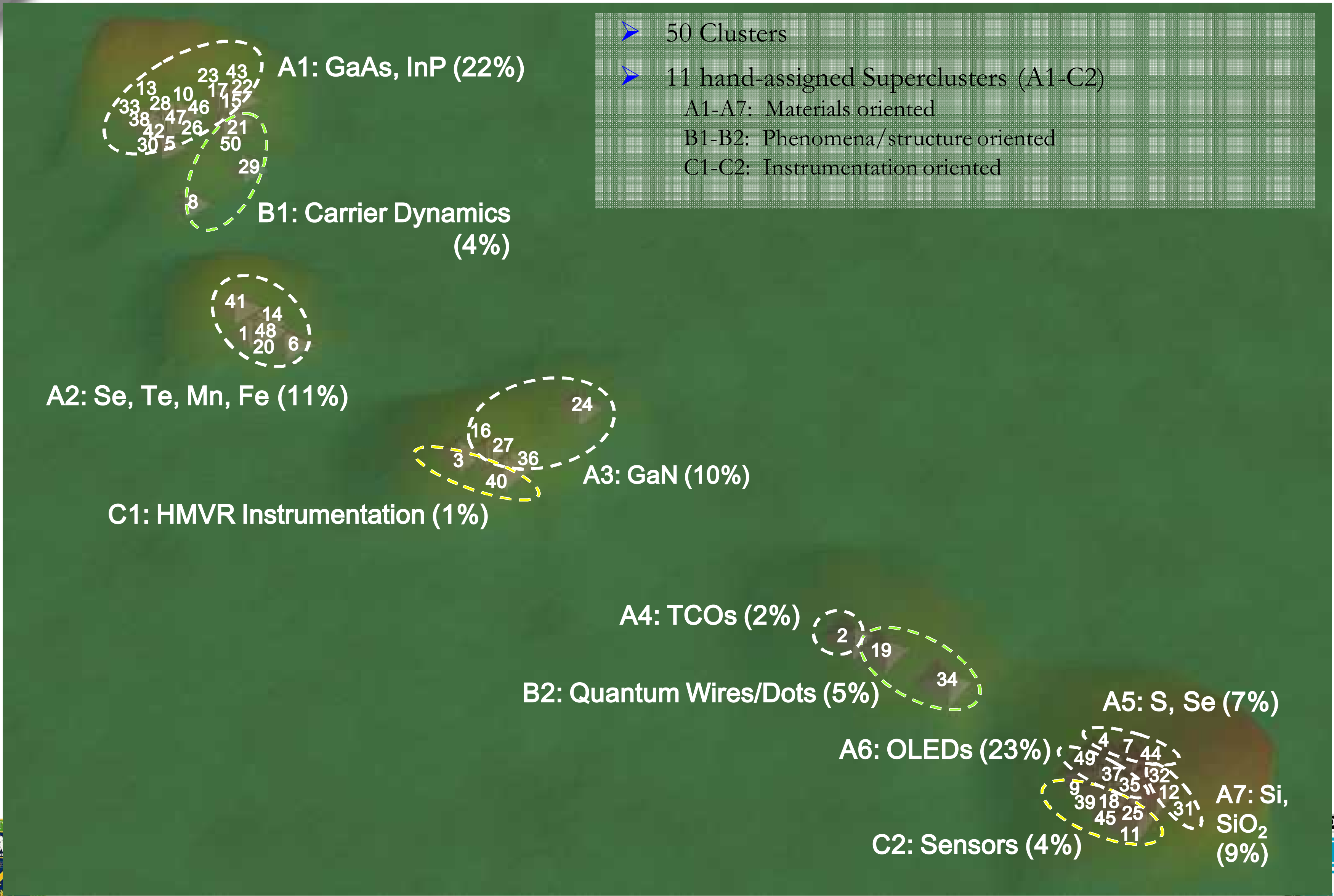
- Boolean search identified 35,000+ papers from 1977 to 2005
- Papers were mapped based on common items in their reference lists
  - Calculate paper-paper similarities
  - Use graph layout tool to determine coordinates
  - Generate cluster assignments based on proximity and edges in the graph
  - Repeat at cluster level …
- 4000+ separate clusters identified
  - Repeated clustering generated ~500 second-level clusters and ~50 third-level clusters
  - 50 third-level clusters were mapped, and 11 high level areas were identified by hand
  - Multi-document summarization was used to extract key phrases for each cluster
- Hot current topics were sought among the 500 second-level clusters
  - Current: mean publication year for cluster > 2000
  - Hot: ratio of actual citations to expected citations > 2.0





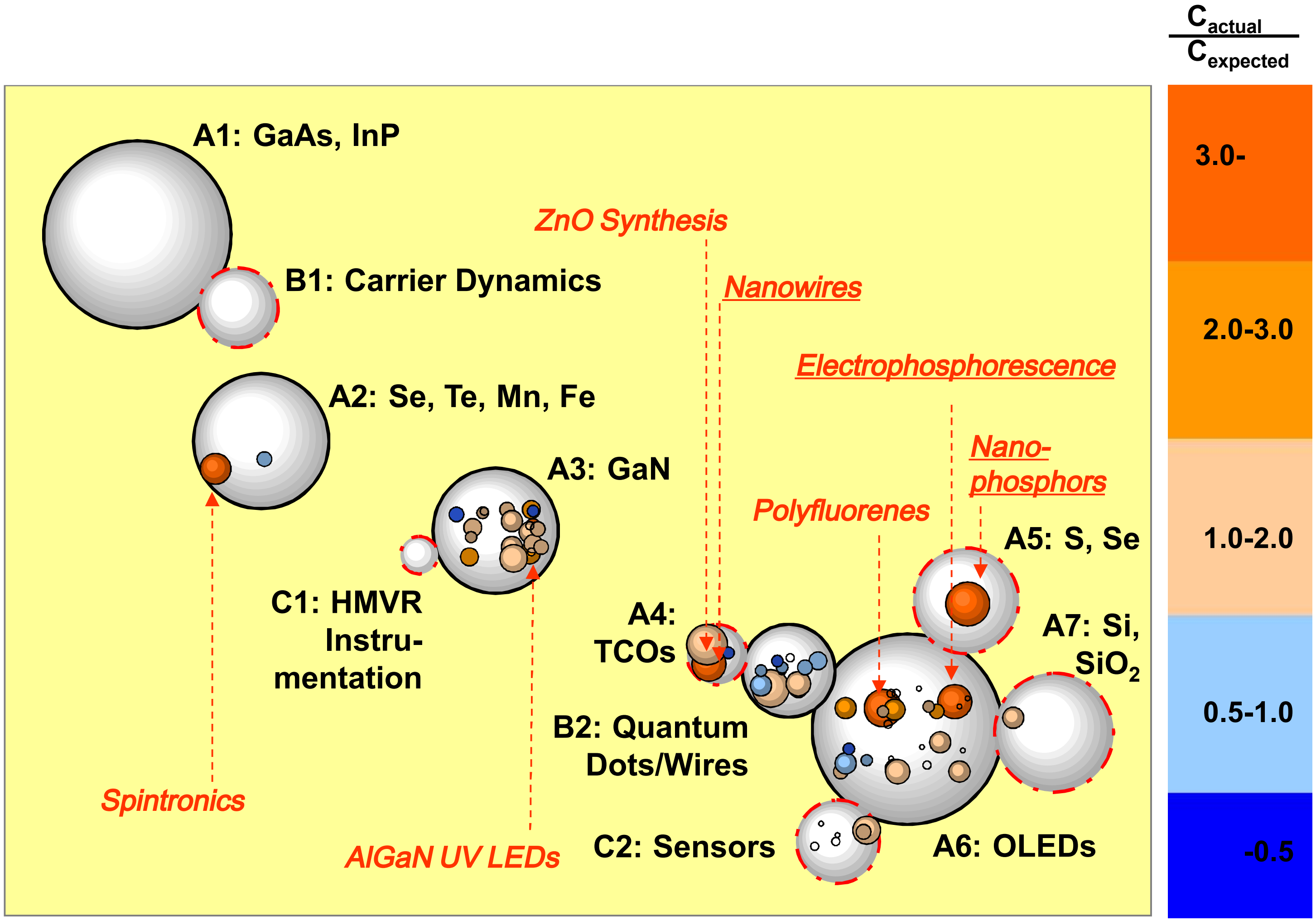


Annotated literature map

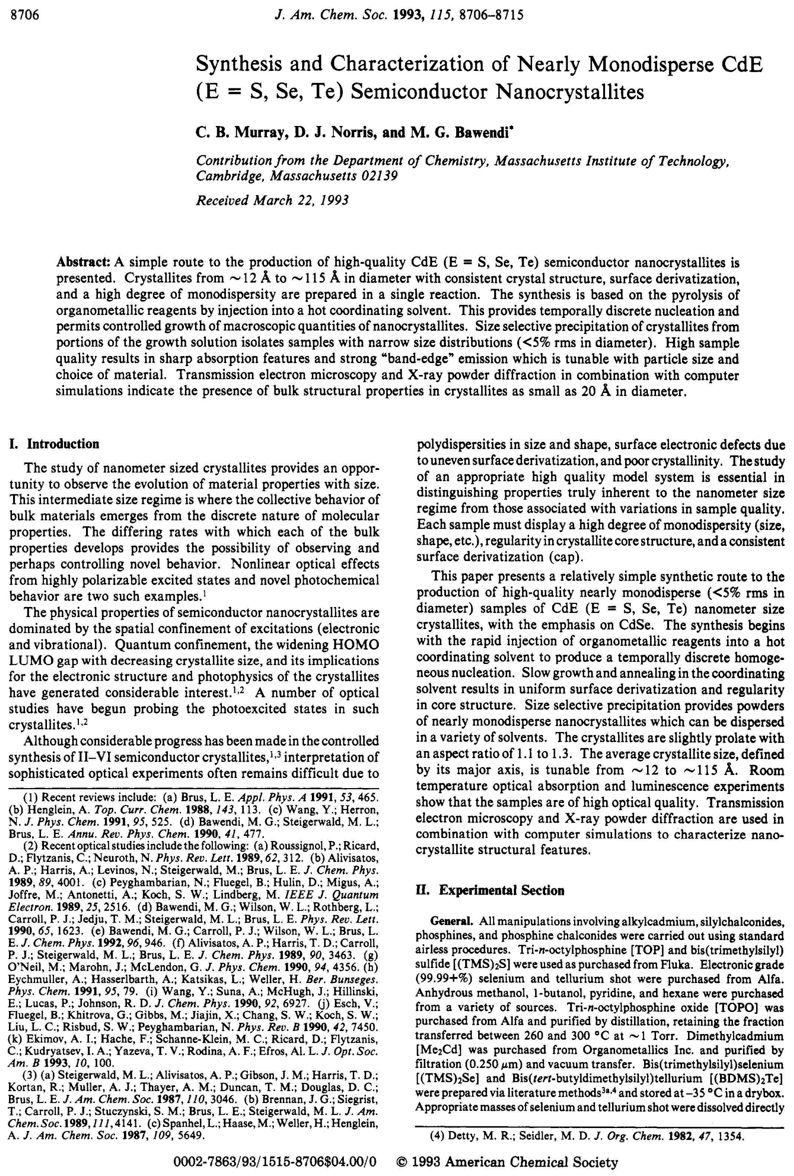


- 50 Clusters
- 11 hand-assigned Superclusters (A1-C2)
  - A1-A7: Materials oriented
  - B1-B2: Phenomena/structure oriented
  - C1-C2: Instrumentation oriented

Hot SSL science clusters



Nanophosphors



8706 J. Am. Chem. Soc. **1993,** *115,* 8706–8715

Synthesis and Characterization of Nearly Monodisperse CdE (E = S, Se, Te) Semiconductor Nanocrystallites

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Abstract: A simple route to the production of high-quality CdE (E = S, Se, Te) semiconductor nanocrystallites is presented. Crystallites from ~12 Å to ~115 Å in diameter with consistent crystal structure, surface derivatization, and a high degree of monodispersity are prepared in a single reaction. The synthesis is based on the pyrolysis of organometallic reagents by injection into a hot coordinating solvent. This provides temporally discrete nucleation and permits controlled growth of macroscopic quantities of nanocrystallites. Size selective precipitation of crystallites from portions of the growth solution isolates samples with narrow size distributions (<5% rms in diameter). High sample quality results in sharp absorption features and strong "band-edge" emission which is tunable with particle size and choice of material. Transmission electron microscopy and X-ray powder diffraction in combination with computer simulations indicate the presence of bulk structural properties in crystallites as small as 20 Å in diameter.

I. Introduction

The study of nanometer sized crystallites provides an opportunity to observe the evolution of material properties with size. This intermediate size regime is where the collective behavior of bulk materials emerges from the discrete nature of molecular properties. The differing rates with which each of the bulk properties develops provides the possibility of observing and perhaps controlling novel behavior. Nonlinear optical effects from highly polarizable excited states and novel photochemical behavior are two such examples.[1]

The physical properties of semiconductor nanocrystallites are dominated by the spatial confinement of excitations (electronic and vibrational). Quantum confinement, the widening HOMO LUMO gap with decreasing crystallite size, and its implications for the electronic structure and photophysics of the crystallites have generated considerable interest.[1,2] A number of optical studies have begun probing the photoexcited states in such crystallites.[1,2]

Although considerable progress has been made in the controlled synthesis of II–VI semiconductor crystallites,[1,3] interpretation of sophisticated optical experiments often remains difficult due to polydispersities in size and shape, surface electronic defects due to uneven surface derivatization, and poor crystallinity. The study of an appropriate high quality model system is essential in distinguishing properties truly inherent to the nanometer size regime from those associated with variations in sample quality. Each sample must display a high degree of monodispersity (size, shape, etc.), regularity in crystallite core structure, and a consistent surface derivatization (cap).

This paper presents a relatively simple synthetic route to the production of high-quality nearly monodisperse (<5% rms in diameter) samples of CdE (E = S, Se, Te) nanometer size crystallites, with the emphasis on CdSe. The synthesis begins with the rapid injection of organometallic reagents into a hot coordinating solvent to produce a temporally discrete homogeneous nucleation. Slow growth and annealing in the coordinating solvent results in uniform surface derivatization and regularity in core structure. Size selective precipitation provides powders of nearly monodisperse nanocrystallites which can be dispersed in a variety of solvents. The crystallites are slightly prolate with an aspect ratio of 1.1 to 1.3. The average crystallite size, defined by its major axis, is tunable from ~12 to ~115 Å. Room temperature optical absorption and luminescence experiments show that the samples are of high optical quality. Transmission electron microscopy and X-ray powder diffraction are used in combination with computer simulations to characterize nanocrystallite structural features.

II. Experimental Section

General. All manipulations involving alkylcadmium, silylchalconides, phosphines, and phosphine chalconides were carried out using standard airless procedures. Tri-*n*-octylphosphine [TOP] and bis(trimethylsilyl) sulfide [$(TMS)_2S$] were used as purchased from Fluka. Electronic grade (99.99+%) selenium and tellurium shot were purchased from Alfa. Anhydrous methanol, 1-butanol, pyridine, and hexane were purchased from a variety of sources. Tri-*n*-octylphosphine oxide [TOPO] was purchased from Alfa and purified by distillation, retaining the fraction transferred between 260 and 300 °C at ~1 Torr. Dimethylcadmium [Me_2Cd] was purchased from Organometallics Inc. and purified by filtration (0.250 μm) and vacuum transfer. Bis(trimethylsilyl)selenium [$(TMS)_2Se$] and Bis(*tert*-butyldimethylsilyl)tellurium [$(BDMS)_2Te$] were prepared via literature methods[3a,4] and stored at −35 °C in a drybox. Appropriate masses of selenium and tellurium shot were dissolved directly

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(1) Recent reviews include: (a) Brus, L. E. *Appl. Phys. A* **1991**, *53*, 465. (b) Henglein, A. *Top. Curr. Chem.* **1988**, *143*, 113. (c) Wang, Y.; Herron, N. *J. Phys. Chem.* **1991**, *95*, 525. (d) Bawendi, M. G.; Steigerwald, M. L.; Brus, L. E. *Annu. Rev. Phys. Chem.* **1990**, *41*, 477.

(2) Recent optical studies include the following: (a) Roussignol, P.; Ricard, D.; Flytzanis, C.; Neuroth, N. *Phys. Rev. Lett.* **1989**, *62*, 312. (b) Alivisatos, A. P.; Harris, A.; Levinos, N.; Steigerwald, M.; Brus, L. E. *J. Chem. Phys.* **1989**, *89*, 4001. (c) Peyghambarian, N.; Fluegel, B.; Hulin, D.; Migus, A.; Joffre, M.; Antonetti, A.; Koch, S. W.; Lindberg, M. *IEEE J. Quantum Electron.* **1989**, *25*, 2516. (d) Bawendi, M. G.; Wilson, W. L.; Rothberg, L.; Carroll, P. J.; Jedju, T. M.; Steigerwald, M. L.; Brus, L. E. *Phys. Rev. Lett.* **1990**, *65*, 1623. (e) Bawendi, M. G.; Carroll, P. J.; Wilson, W. L.; Brus, L. E. *J. Chem. Phys.* **1992**, *96*, 946. (f) Alivisatos, A. P.; Harris, T. D.; Carroll, P. J.; Steigerwald, M. L.; Brus, L. E. *J. Chem. Phys.* **1989**, *90*, 3463. (g) O'Neil, M.; Marohn, J.; McLendon, G. *J. Phys. Chem.* **1990**, *94*, 4356. (h) Eychmuller, A.; Hasserlbarth, A.; Katsikas, L.; Weller, H. *Ber. Bunseges. Phys. Chem.* **1991**, *95*, 79. (i) Wang, Y.; Suna, A.; McHugh, J.; Hillinski, E.; Lucas, P.; Johnson, R. D. *J. Chem. Phys.* **1990**, *92*, 6927. (j) Esch, V.; Fluegel, B.; Khitrova, G.; Gibbs, M.; Jiajin, X.; Chang, S. W.; Koch, S. W.; Liu, L. C.; Risbud, S. W.; Peyghambarian, N. *Phys. Rev. B* **1990**, *42*, 7450. (k) Ekimov, A. I.; Hache, F.; Schanne-Klein, M. C.; Ricard, D.; Flytzanis, C.; Kudryatsev, I. A.; Yazeva, T. V.; Rodina, A. F.; Efros, Al. L. *J. Opt. Soc. Am. B* **1993**, *10*, 100.

(3) (a) Steigerwald, M. L.; Alivisatos, A. P.; Gibson, J. M.; Harris, T. D.; Kortan, R.; Muller, A. J.; Thayer, A. M.; Duncan, T. M.; Douglas, D. C.; Brus, L. E. *J. Am. Chem. Soc.* **1987**, *110*, 3046. (b) Brennan, J. G.; Siegrist, T.; Carroll, P. J.; Stuczynski, S. M.; Brus, L. E.; Steigerwald, M. L. *J. Am. Chem. Soc.* **1989**, *111*, 4141. (c) Spanhel, L.; Haase, M.; Weller, H.; Henglein, A. *J. Am. Chem. Soc.* **1987**, *109*, 5649.

(4) Detty, M. R.; Seidler, M. D. *J. Org. Chem.* **1982**, *47*, 1354.

0002-7863/93/1515-8706$04.00/0

- 1993-94 breakthrough (MIT, UC Berkeley):
  - precipitation technique for monodisperse CdSe nanocrystals
  - observation of high photoluminescence efficiencies and quantum size effects
- Since then, great interest in:
  - multi-step synthesis of "core-shell" nanocrystals
  - extending range of semiconducting materials and emission wavelengths
  - polymer/nanocrystal devices
- Promise:
  - Ultrasensitive biomolecular assays (e.g., antibodies, RNA)
  - Tunable scatter-free wavelength downconversion
  - Hybrid inorganic/organic LEDs

Electrophosphorescence

Highly efficient phosphorescent emission from organic electroluminescent devices

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† *Department of Chemistry, University of Southern California, Los Angeles, California 90089, USA*

The efficiency of electroluminescent organic light-emitting devices[1,2] can be improved by the introduction[3] of a fluorescent dye. Energy transfer from the host to the dye occurs via excitons, but only the singlet spin states induce fluorescent emission; these represent a small fraction (about 25%) of the total excited-state population (the remainder are triplet states). Phosphorescent dyes, however, offer a means of achieving improved light-emission efficiencies, as emission may result from both singlet and triplet states. Here we report high-efficiency ($\geqslant$ 90%) energy transfer from both singlet and triplet states, in a host material doped with the phosphorescent dye 2,3,7,8,12,13,17,18-octaethyl-21H,23H-porphine platinum(II) (PtOEP). Our doped electroluminescent devices generate saturated red emission with peak external and internal quantum efficiencies of 4% and 23%, respectively. The luminescent efficiencies attainable with phosphorescent dyes may lead to new applications for organic materials. Moreover, our work establishes the utility of PtOEP as a probe of triplet behaviour and energy transfer in organic solid-state systems.

When the absorption spectrum of the acceptor (dye) overlaps the emission spectrum of the donor (host), efficient energy transfer from the host to the dye can occur via a singlet-allowed, induced-dipole coupling between the molecular species. Hence, for a fluorescent emitter, the maximum external quantum efficiency (photons extracted in the forward direction per electron injected) is[4,5]:

$$\Phi_{\mathrm{el}} = \chi \Phi_{\mathrm{fl}} \eta_{\mathrm{r}} \eta_{\mathrm{e}}$$

The fraction of charge carrier recombinations in the host resulting in singlet excitons is χ, which from spin statistics is presumed to be ~1/4, Φ_{fl} is the photoluminescent efficiency of the dye, η_{e} is the fraction of emitted photons that are coupled out of the device, and η_{r} is the fraction of injected charge carriers that form excitons. As both the recombination and fluorescent efficiencies can approach unity for an optimized device, the efficiency is primarily limited by coupling losses and a restriction to singlet excitons imposed by spin conservation in the induced-dipole energy-transfer process.

Although the output coupling of photons can be increased by using shaped substrates[6], further efficiency improvements require that both singlet and triplet excited states contribute to luminescence. It has been proposed that intersystem crossing in lanthanide complexes may achieve this with an intramolecular energy transfer from a triplet state of the organic ligand to the 4*f* energy state of the ion[7]. However, a more general and efficient solution to the problem is to use phosphorescent emissive materials.

Phosphorescence is the forbidden relaxation of an excited state with spin symmetry different from the ground state; in organic molecules it typically results from a triplet to a singlet relaxation. Although low-efficiency electroluminescence has been demonstrated[8] at 100 K using the phosphorescent material benzophenone doped into poly(methylmethacrylate), no energy transfer from the host material was found. If a phosphorescent dye participates in energy transfer, then triplet behaviour within the host can be directly examined. This may enable the accurate determination of spin statistics and other triplet properties, as well as resulting in very high electroluminescent efficiency devices.

One relatively well studied red emitting phosphorescent dye is PtOEP. Porphine complexes are known to possess long-lived triplet states useful in oxygen detection[9]. The addition of platinum to the porphine ring reduces the phosphorescence lifetime by increasing spin–orbit coupling; the triplet states gain additional singlet character and vice versa. This also enhances the efficiency of intersystem crossing from the first singlet excited state to the triplet excited state. Transient absorption spectrometry gives a singlet lifetime in PtOEP of ~1 ps, and the fluorescence efficiency is extremely weak[10]. In contrast, the room-temperature phosphorescence efficiency of PtOEP in a polystyrene matrix is[11] 0.5 with an observed lifetime of 91 μs.

Induced dipole (or Förster) energy transfer to the triplet state is disallowed by spin conservation. However, energy transfer may occur by the parallel combination of Förster transfer to the singlet state, along with electron exchange (Dexter energy transfer). Dexter transfer is the 'physical', coherent transfer of an exciton from a donor to an acceptor site[12] at a rate proportional to the orbital overlap of the donor and acceptor molecules. Consequently, it is a short-range process, attenuating exponentially with distance. The transfer rate is proportional to the spectral overlap of the two species because the donor exciton energy must closely match that of the acceptor. Dexter processes allow for the transfer of triplet excitons because only the total spin of the donor–acceptor complex is conserved. Thus it is possible for both singlets and triplets to excite phosphorescence, increasing the theoretical efficiency limit from that for fluorescence by a factor of four or larger.

PtOEP shows[13] strong absorption at a wavelengths of 530 nm, corresponding to the peak emission of the electron transport material, tris-(8-hydroxyquinoline) aluminium (Alq_3); this makes PtOEP a suitable dopant for Alq_3-based organic light-emitting diodes (LEDs). To study the electroluminescent properties of Alq_3/PtOEP systems, organic LEDs were produced by high-vacuum (10^{-6} torr) thermal evaporation onto a cleaned glass substrate precoated with conductive, transparent indium tin oxide (ITO). The test structure consists of a 60-Å-thick layer of copper phthalocyanine to aid hole injection from the ITO, a 350-Å-thick layer of the hole transporting material 4,4′-bis[N-(1-napthyl)-N-phenyl-amino] biphenyl (α-NPD), a 400-Å-thick layer of Alq_3 doped with varying molar concentrations of PtOEP, and a further 100-Å-thick layer of Alq_3 to prevent quenching of PtOEP excitons at the cathode. Finally, a shadow mask with 1-mm-diameter openings was used to define the cathode consisting of a 1,000-Å-thick layer of 25:1 Mg:Ag, with a 500-Å-thick Ag cap. All measurements were performed in air at room temperature except for the photoluminescence measurements which were performed under nitrogen.

The electroluminescence spectra of the devices with three different concentrations of PtOEP are shown in Fig. 1. No significant emission is found for the previously identified singlet state, expected at ~580 nm (ref. 10), but strong emission is observed from the triplet excited state at 650 nm, with weaker emission seen at the vibronic harmonic overtones at 623 nm, 687 nm and 720 nm. At high drive currents, the emission at 650 nm saturates, and increasing emission is seen from other features, especially the broad Alq_3 peak centred at 530 nm. This results in a reversible shift in colour from deep red to orange, corresponding to a shift in the device chromaticity co-ordinates shown in Fig. 1 inset.

Spectral and time-resolved emission measurements were performed with a streak camera on our organic LEDs excited with current pulses. Slow decay of between 10 and 50 μs was observed for

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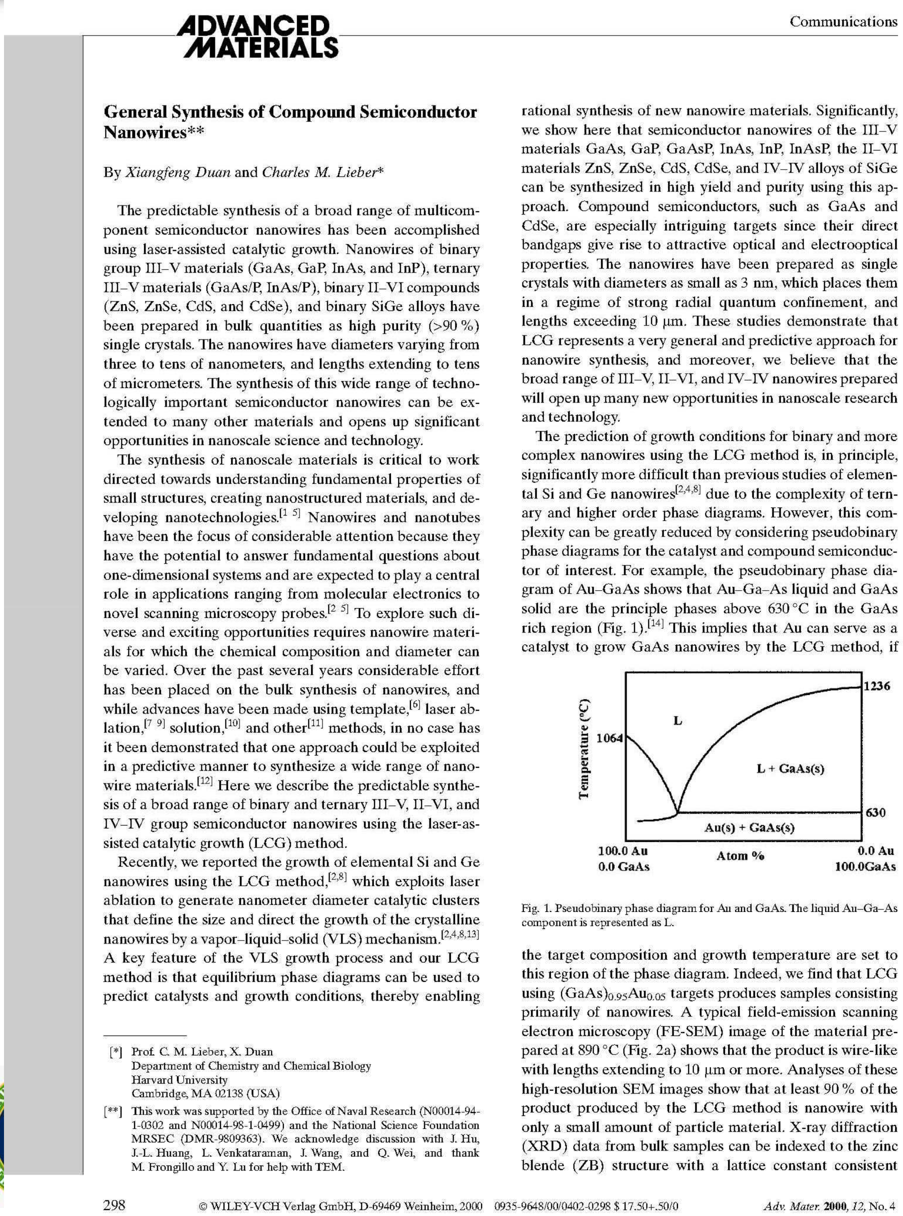
‡ Permanent address: Department of Chemistry, Goucher College, Baltimore, Maryland 21204-2794, USA.

- 1998 breakthrough (Princeton):
  - – efficient light emission from triplet states of phosphorescent dye in Alq3 host
- Since then, great interest in:
  - – optimizing host/dye combinations for host-to-dye energy transfer and subsequent light emission
  - – extension to blue
  - – extension to polymers
- Promise:
  - – Improve the previous 25% limit on quantum efficiency from singlet states alone to 100%

Nanowires



ADVANCED MATERIALS

General Synthesis of Compound Semiconductor Nanowires**

By *Xiangfeng Duan* and *Charles M. Lieber**

The predictable synthesis of a broad range of multicomponent semiconductor nanowires has been accomplished using laser-assisted catalytic growth. Nanowires of binary group III–V materials (GaAs, GaP, InAs, and InP), ternary III–V materials (GaAs/P, InAs/P), binary II–VI compounds (ZnS, ZnSe, CdS, and CdSe), and binary SiGe alloys have been prepared in bulk quantities as high purity (>90 %) single crystals. The nanowires have diameters varying from three to tens of nanometers, and lengths extending to tens of micrometers. The synthesis of this wide range of technologically important semiconductor nanowires can be extended to many other materials and opens up significant opportunities in nanoscale science and technology.

The synthesis of nanoscale materials is critical to work directed towards understanding fundamental properties of small structures, creating nanostructured materials, and developing nanotechnologies.[1 5] Nanowires and nanotubes have been the focus of considerable attention because they have the potential to answer fundamental questions about one-dimensional systems and are expected to play a central role in applications ranging from molecular electronics to novel scanning microscopy probes.[2 5] To explore such diverse and exciting opportunities requires nanowire materials for which the chemical composition and diameter can be varied. Over the past several years considerable effort has been placed on the bulk synthesis of nanowires, and while advances have been made using template,[6] laser ablation,[7 9] solution,[10] and other[11] methods, in no case has it been demonstrated that one approach could be exploited in a predictive manner to synthesize a wide range of nanowire materials.[12] Here we describe the predictable synthesis of a broad range of binary and ternary III–V, II–VI, and IV–IV group semiconductor nanowires using the laser-assisted catalytic growth (LCG) method.

Recently, we reported the growth of elemental Si and Ge nanowires using the LCG method,[2,8] which exploits laser ablation to generate nanometer diameter catalytic clusters that define the size and direct the growth of the crystalline nanowires by a vapor–liquid–solid (VLS) mechanism.[2,4,8,13] A key feature of the VLS growth process and our LCG method is that equilibrium phase diagrams can be used to predict catalysts and growth conditions, thereby enabling rational synthesis of new nanowire materials. Significantly, we show here that semiconductor nanowires of the III–V materials GaAs, GaP, GaAsP, InAs, InP, InAsP, the II–VI materials ZnS, ZnSe, CdS, CdSe, and IV–IV alloys of SiGe can be synthesized in high yield and purity using this approach. Compound semiconductors, such as GaAs and CdSe, are especially intriguing targets since their direct bandgaps give rise to attractive optical and electrooptical properties. The nanowires have been prepared as single crystals with diameters as small as 3 nm, which places them in a regime of strong radial quantum confinement, and lengths exceeding 10 μm. These studies demonstrate that LCG represents a very general and predictive approach for nanowire synthesis, and moreover, we believe that the broad range of III–V, II–VI, and IV–IV nanowires prepared will open up many new opportunities in nanoscale research and technology.

The prediction of growth conditions for binary and more complex nanowires using the LCG method is, in principle, significantly more difficult than previous studies of elemental Si and Ge nanowires[2,4,8] due to the complexity of ternary and higher order phase diagrams. However, this complexity can be greatly reduced by considering pseudobinary phase diagrams for the catalyst and compound semiconductor of interest. For example, the pseudobinary phase diagram of Au–GaAs shows that Au–Ga–As liquid and GaAs solid are the principle phases above 630 °C in the GaAs rich region (Fig. 1).[14] This implies that Au can serve as a catalyst to grow GaAs nanowires by the LCG method, if the target composition and growth temperature are set to this region of the phase diagram. Indeed, we find that LCG using $(GaAs)_{0.95}Au_{0.05}$ targets produces samples consisting primarily of nanowires. A typical field-emission scanning electron microscopy (FE-SEM) image of the material prepared at 890 °C (Fig. 2a) shows that the product is wire-like with lengths extending to 10 μm or more. Analyses of these high-resolution SEM images show that at least 90 % of the product produced by the LCG method is nanowire with only a small amount of particle material. X-ray diffraction (XRD) data from bulk samples can be indexed to the zinc blende (ZB) structure with a lattice constant consistent

Fig. 1. Pseudobinary phase diagram for Au and GaAs. The liquid Au–Ga–As component is represented as L.

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- 2000 breakthrough (Harvard):
  - extension of vapor-liquid-solid (VLS) technique to compound semiconductor nanowires
- Since then, great interest in:
  - further extension to wide range of compound semiconductors (e.g., GaN, ZnO)
  - nanowire devices (e.g., nanowire LEDs)
- Promise:
  - Nanoelectronics and Nanophotonics
  - Unconstrained defect-free crystals
  - Higher extraction efficiency LEDs

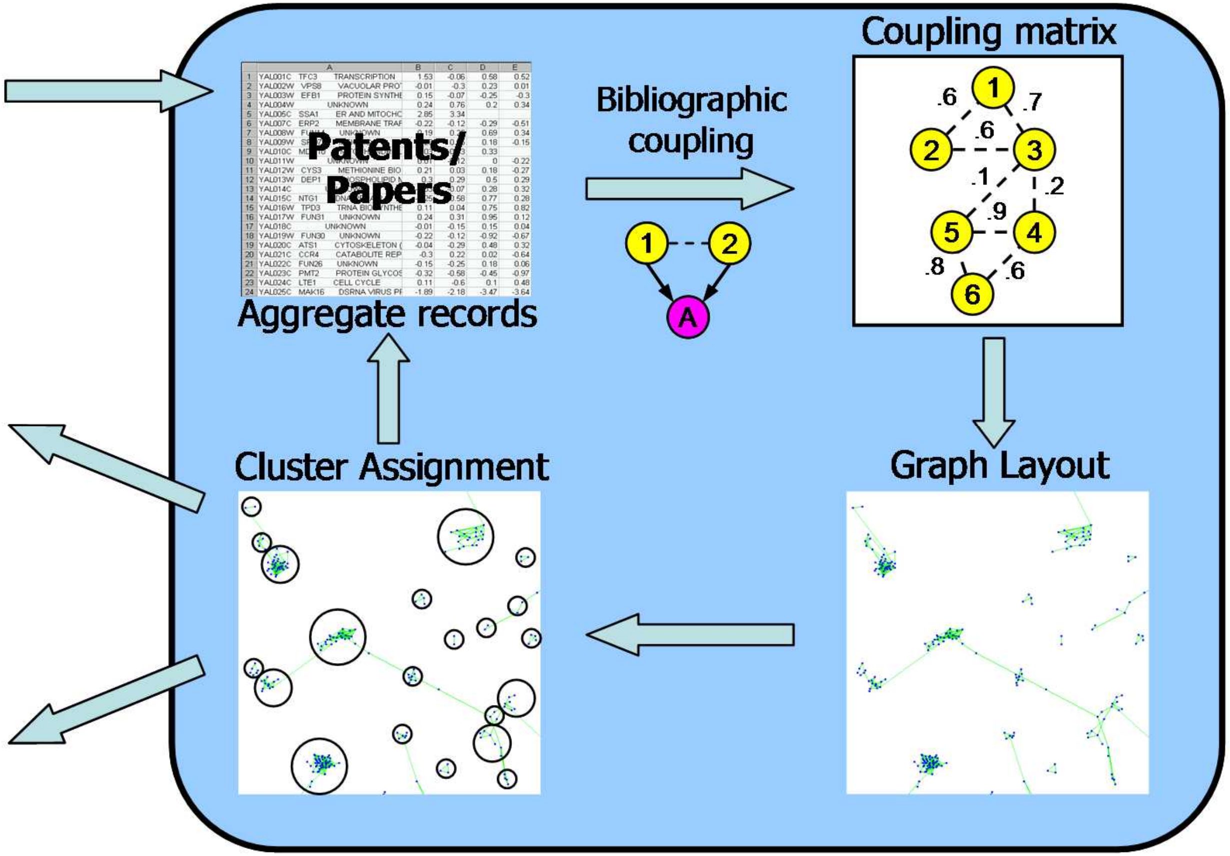
Example 3

Is my niche in bionanotechnology likely to produce commercial results?

- Mapping all of science

Mapping all of science

Search Databases

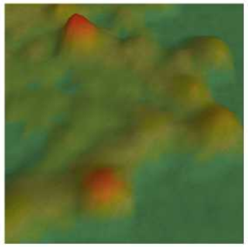


	A	B	C	D	E
1	YAL001C TFC3 TRANSCRIPTION	1.53	-0.06	0.58	0.52
2	YAL002W VPS8 VACUOLAR PRO	-0.01	-0.3	0.23	0.01
3	YAL003W EFB1 PROTEIN SYNTHE	0.15	-0.07	-0.25	-0.3
4	YAL004W UNKNOWN	0.24	0.76	0.2	0.34
5	YAL005C SSA1 ER AND MITOCHC	2.85	3.34		
6	YAL007C ERP2 MEMBRANE TRAF	-0.22	-0.12	-0.29	-0.51
7	YAL008W [illegible] UNKNOWN	[illegible]	[illegible]	0.69	0.34
8	YAL009W [illegible]	[illegible]	[illegible]	0.18	-0.15
9	YAL010C [illegible]	[illegible]	[illegible]	0.33	
10	YAL011W UNKNOWN	[illegible]	[illegible]	0	-0.22
11	YAL012W CYS3 METHIONINE BIO	0.21	0.03	0.18	-0.27
12	YAL013W DEP1 [illegible]	0.3	0.29	0.5	0.29
13	YAL014C [illegible]	[illegible]	[illegible]	0.28	0.32
14	YAL015C NTG1 [illegible]	[illegible]	[illegible]	0.77	0.28
15	YAL016W TPD3 [illegible]	0.11	0.04	0.75	0.82
16	YAL017W FUN31 UNKNOWN	0.24	0.31	0.95	0.12
17	YAL018C UNKNOWN	-0.01	-0.15	0.15	0.04
18	YAL019W FUN30 UNKNOWN	-0.22	-0.12	-0.92	-0.67
19	YAL020C ATS1 CYTOSKELETON (	-0.04	-0.29	0.48	0.32
20	YAL021C CCR4 CATABOLITE REP	-0.3	0.22	0.02	-0.64
21	YAL022C FUN26 UNKNOWN	-0.15	-0.25	0.18	0.06
22	YAL023C PMT2 PROTEIN GLYCOS	-0.32	-0.58	-0.45	-0.97
23	YAL024C LTE1 CELL CYCLE	0.11	-0.6	0.1	0.48
24	YAL025C MAK16 DSRNA VIRUS PI	-1.89	-2.18	-3.47	-3.64

Emergent categories

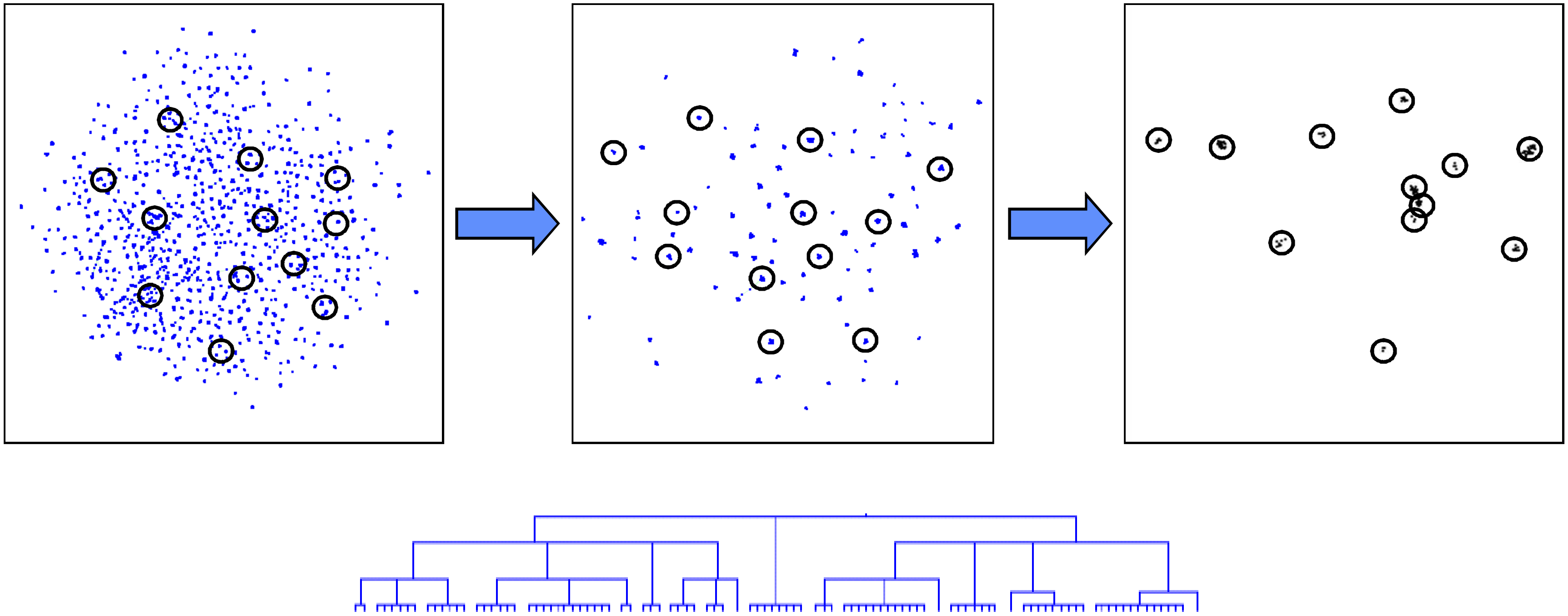
	cluster			
patent_no	lev1	lev2	lev3	lev4
US6821009	1542	368	56	5
US6821143	2273	332	2	2
US6821553	98	258	3	1
US6821643	2286	307	33	1
US6821644				
US6821647	284	187	47	3
US6821648	2173	307	33	1
US6821649	652	289	33	1
US6821650	2015	309	33	1
US6821651	2015	309	33	1
US6821793	2295	95	19	3
US6821799	2252	372	2	2
US6821800	832	334	47	3
US6821803	1965	339	1	1
US6821804	1700	188	58	2
US6821806	1993	279	47	3

Browsable MAPs



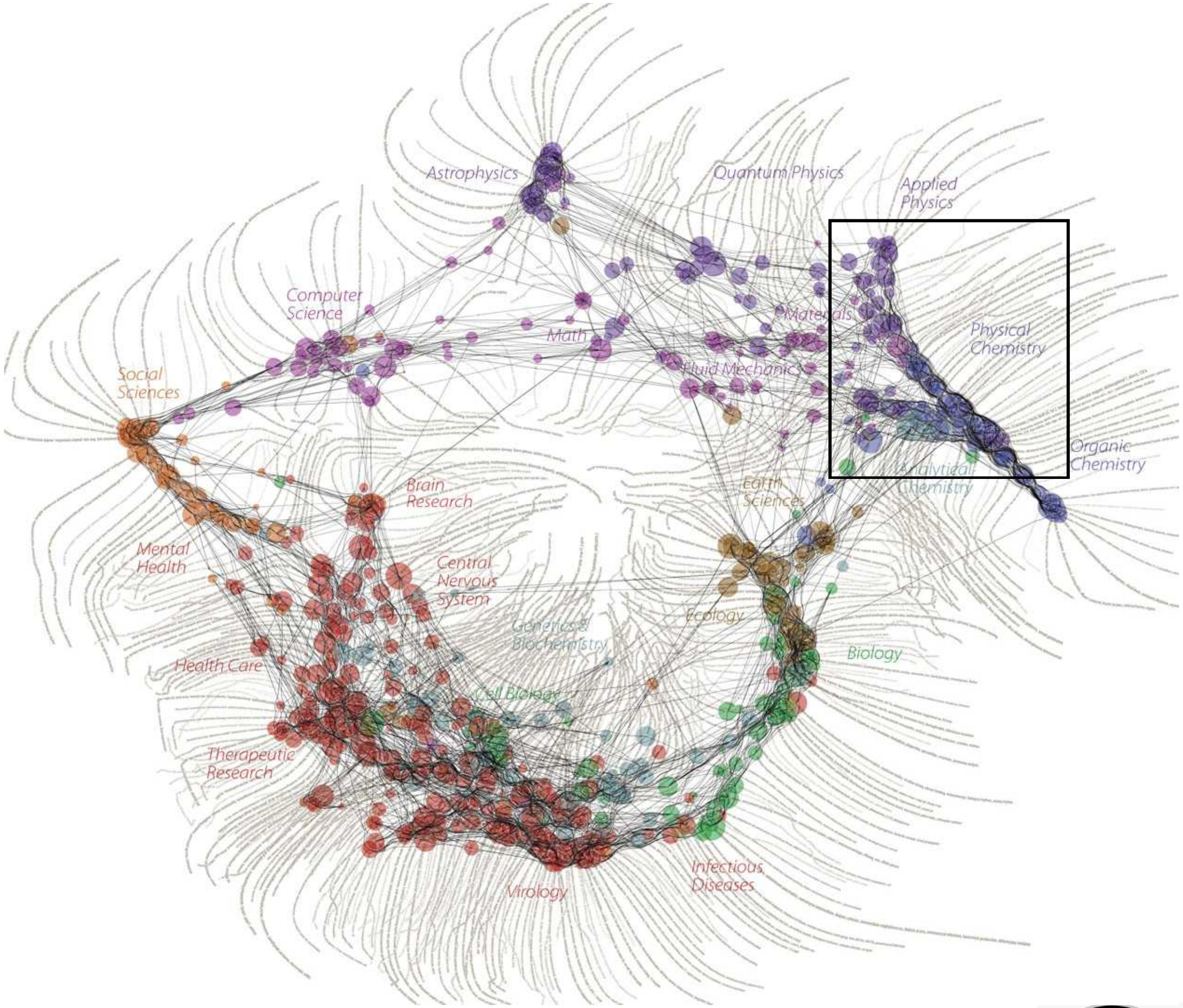
Successive Clusterings

- Iteratively use graph layout and modified single-link to do nested clustering

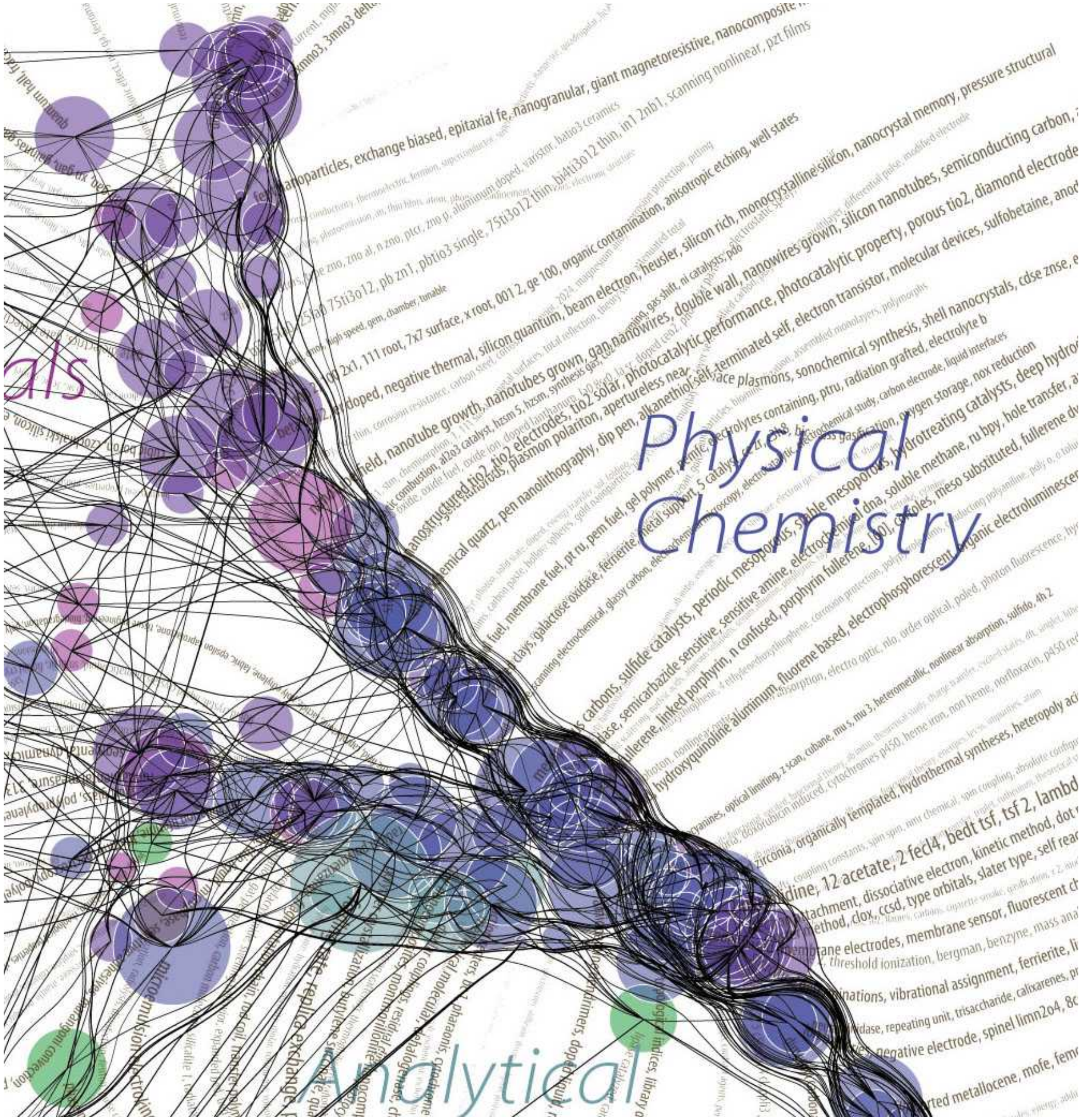


Representative model

- Combined SCIE/ SSCI
- 3 levels of clustering used
  - 820k reference papers
  - 53k communities
  - 6100 level1 clusters
  - 776 paradigms
  - 760k current papers
- Gives a structure of scientific paradigms rather than disciplines
- Indicators calculated at the "community" level
- Aggregated results displayed at the "paradigm" level



Zoomed version



Additional features

- Extract key phrases from level1 clusters
- Additional text-based data can then be probabilistically mapped to clusters
  - Patents, grants, corporate documents, etc.
- 150k patents from 2005
  - retrospective – which clusters have already shown strong linkage to current patents, thus commercial potential
- 180k grants from 2005
  - prospective – which clusters are currently getting large amounts of government funding

Starting point for analysis

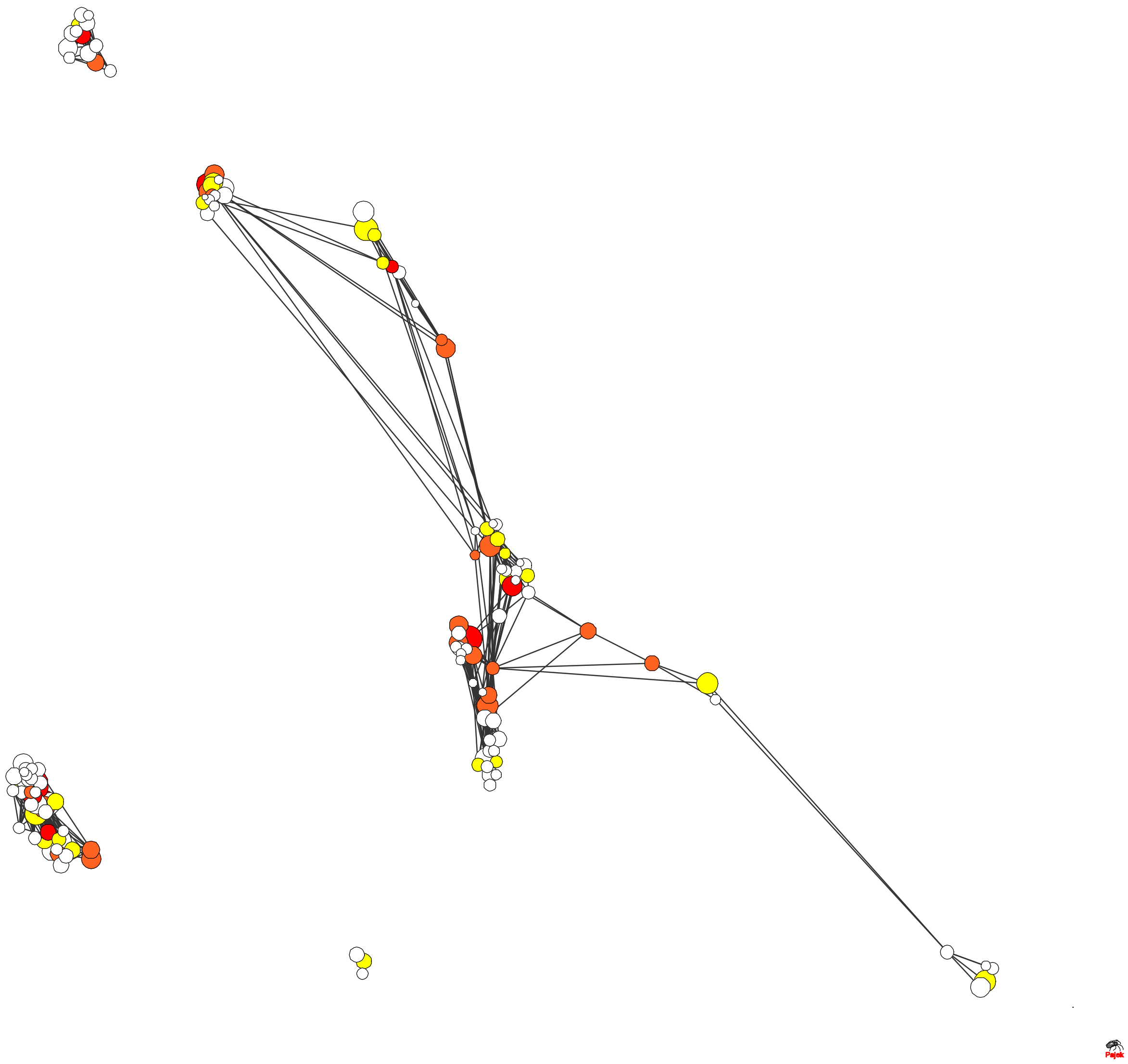
Question: Is my niche in bionanotechnology likely to produce commercial results?

- Seed papers
  - 4-5 papers from most current model year
  - 4-5 most key older references
- Find clusters with seed papers > seed clusters
- Find clusters that are highly linked to seed clusters
  - Dump key phrases from seed and linked cluster
- SME then examines the phrases from each cluster and ranks them as YES, Probably Yes, Probably No, NO (15 minutes)
- Iterate on YES and Probably Yes answers
  - Dump key phrases from YES, Probably, and linked clusters
  - SME ranks clusters again
- Resulting YES, Probably YES answers used as field definition
- Total SME time to this point – typically less than one hour

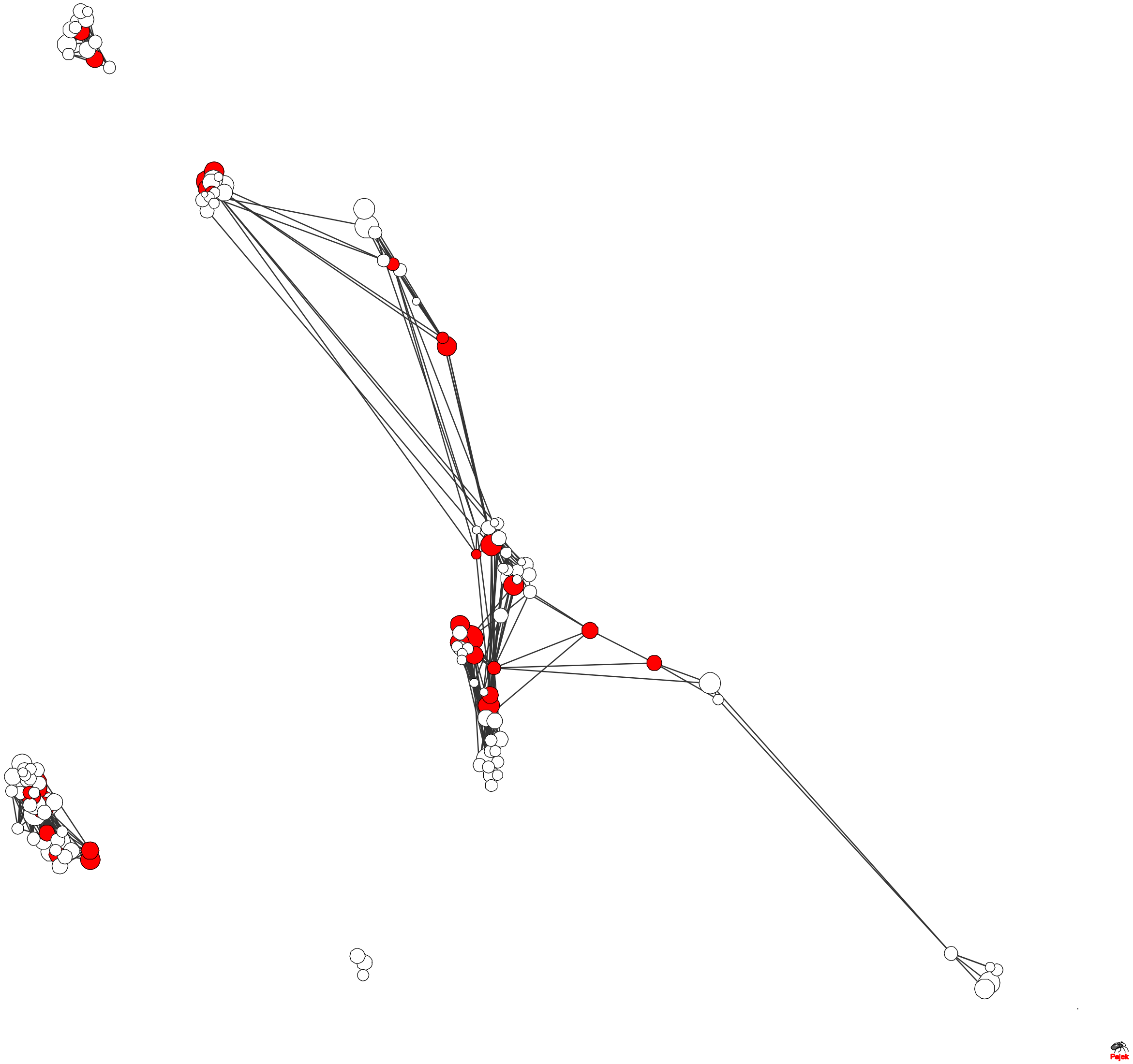
Analysis and reporting

- Extract all clusters (YES, Prob Yes, Prob No, NO) from the overall map
- Extract additional information by cluster
  - Patent counts, patent impact, grant counts, grant amounts
- Create visuals

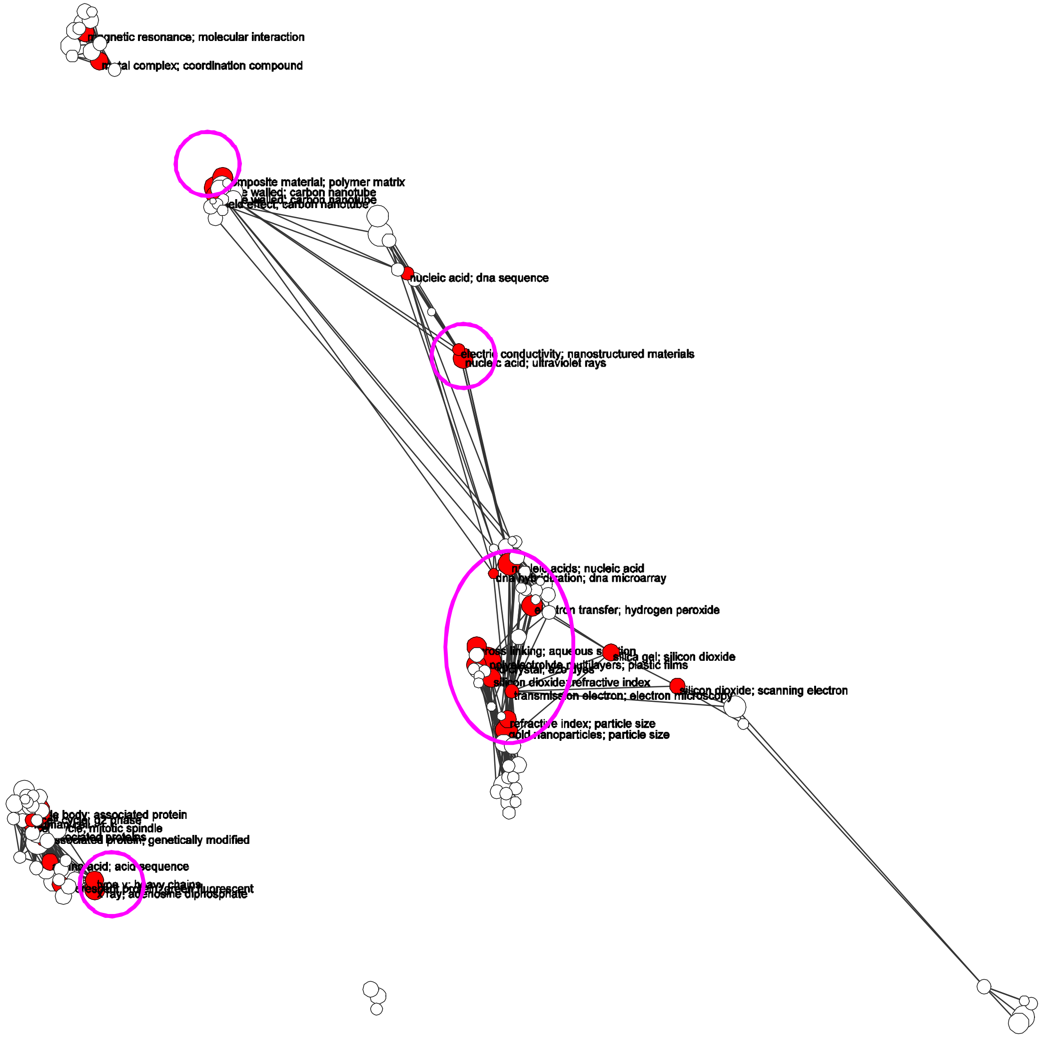
Communities of interest



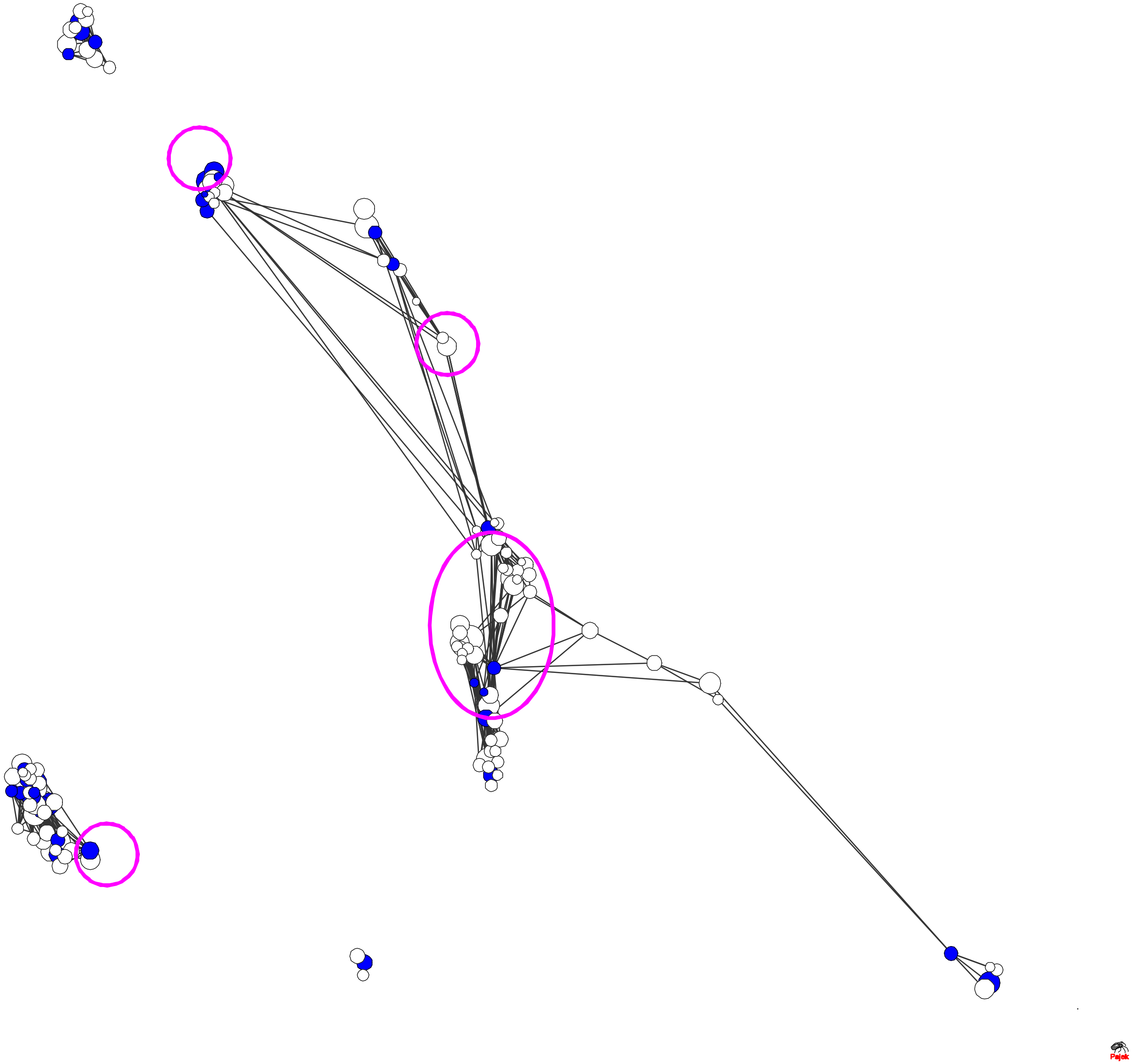
Communities of interest



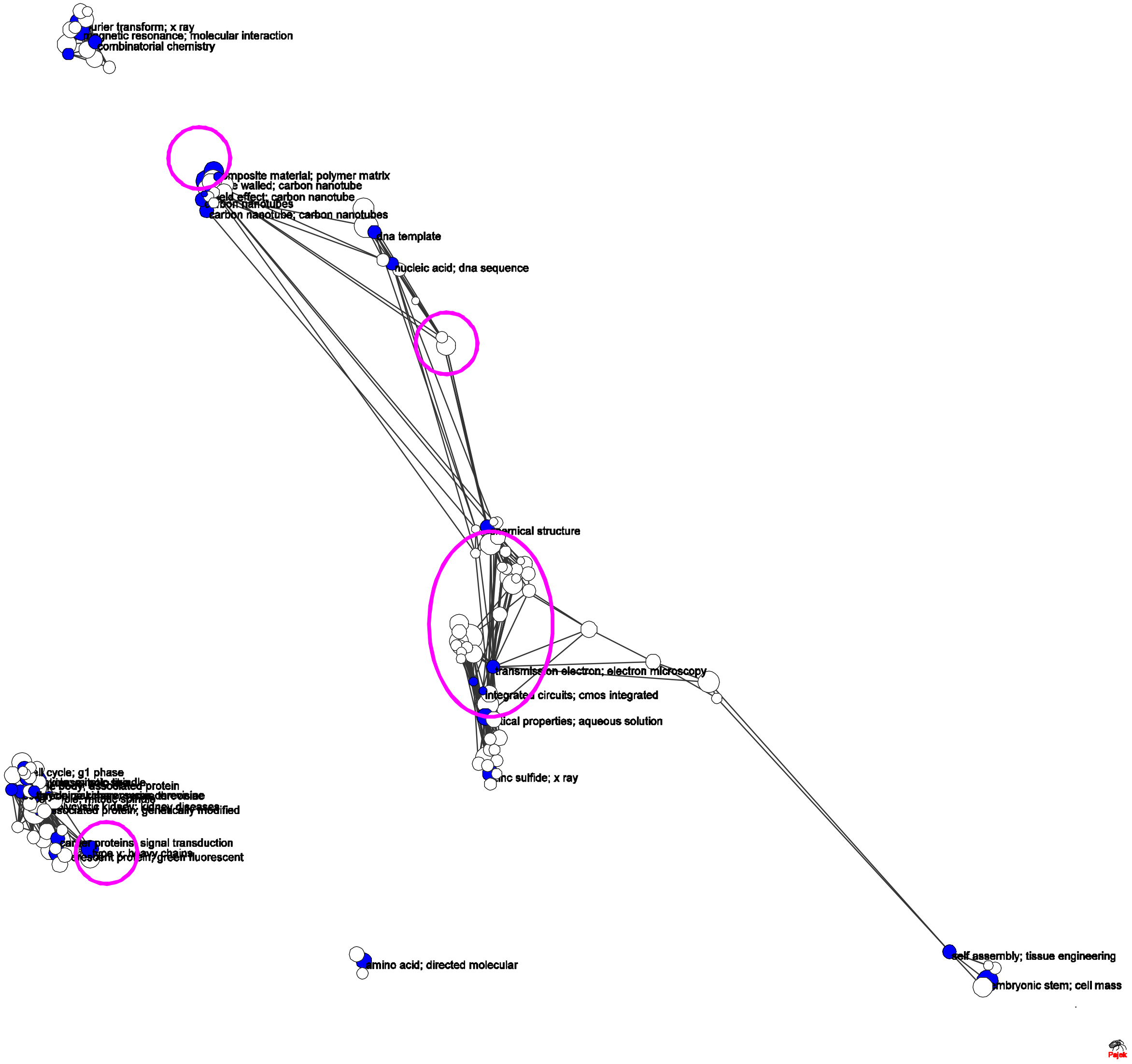
Communities of interest



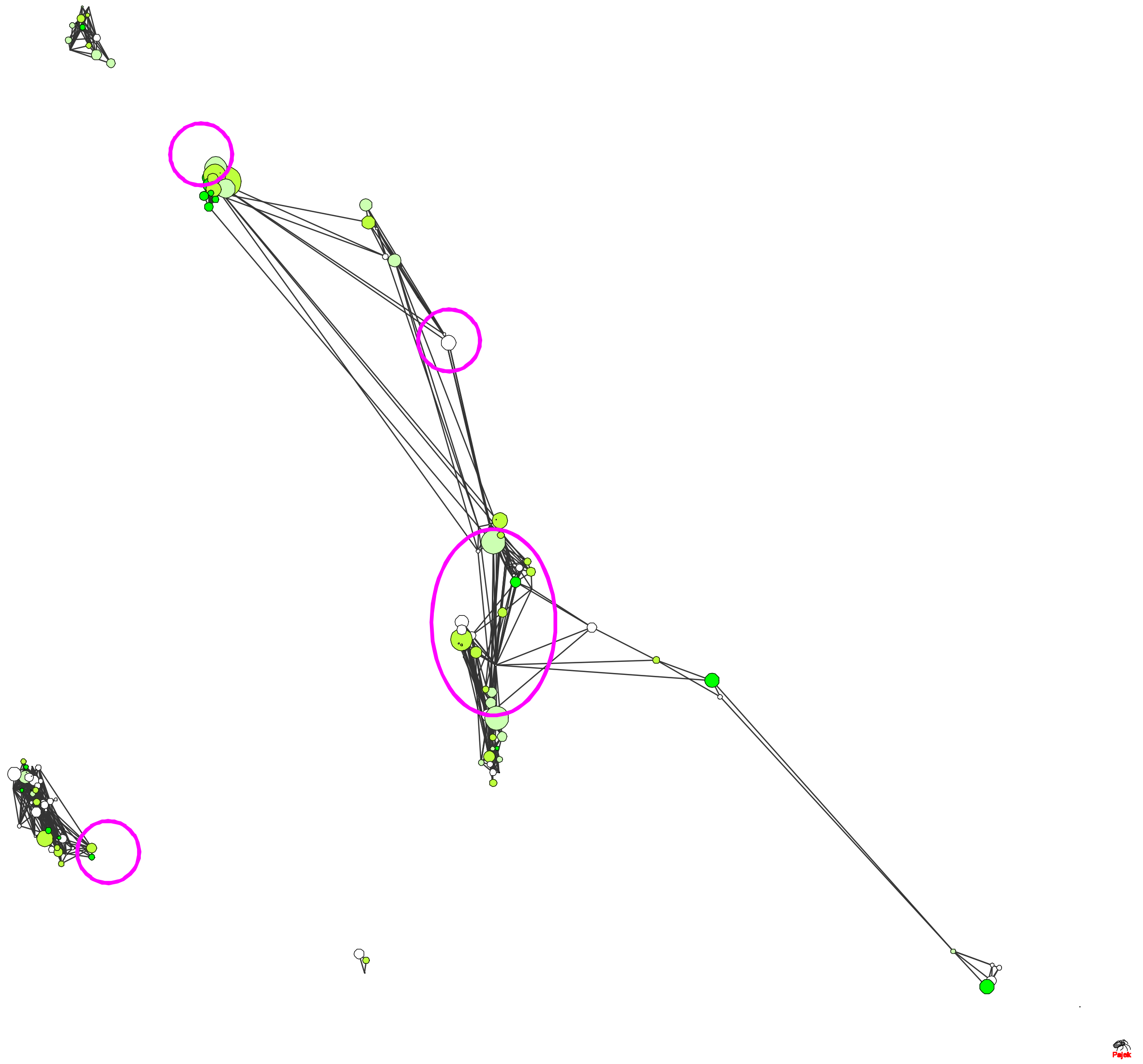
High vitality – fast-moving science



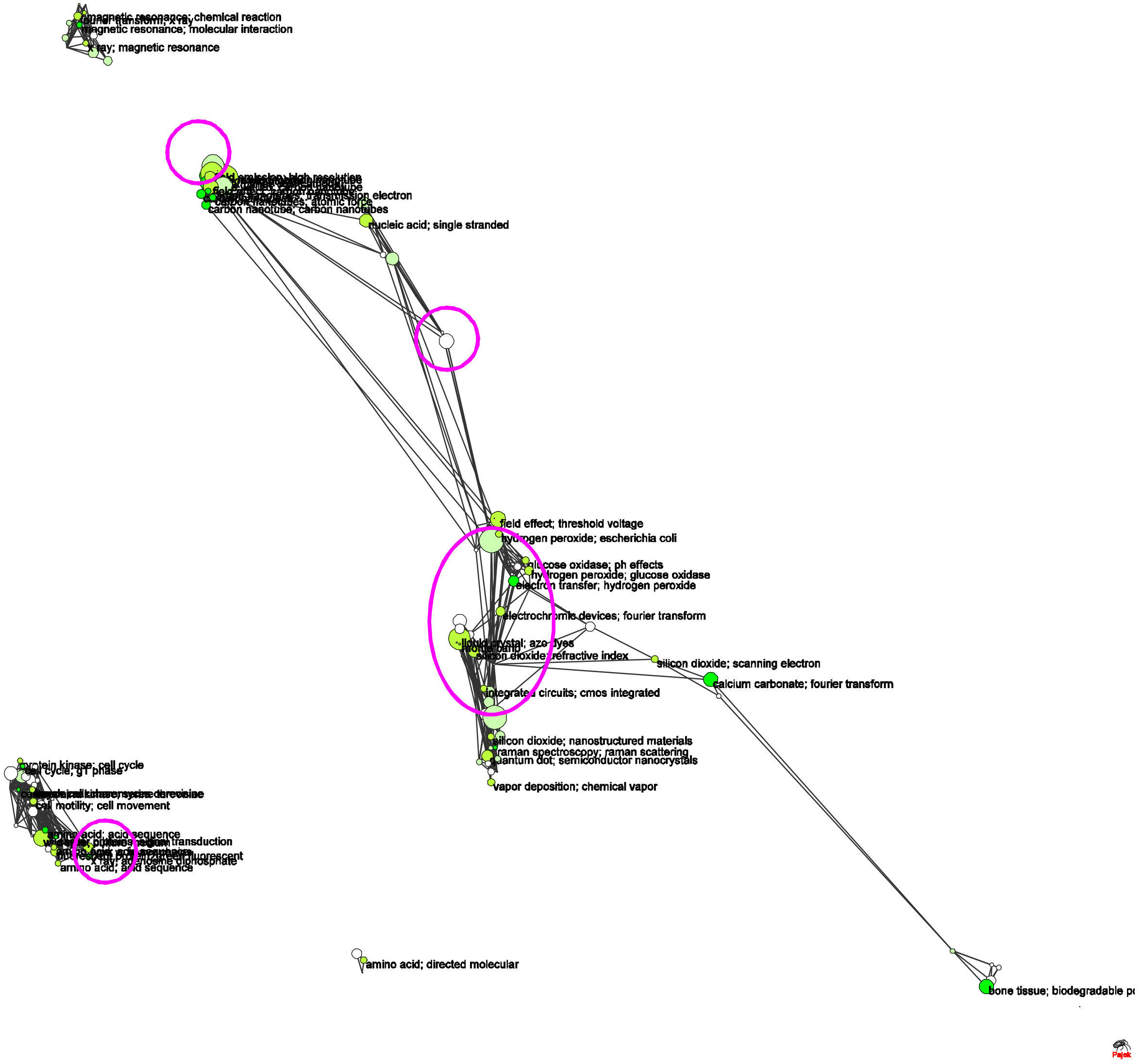
High vitality – fast-moving science



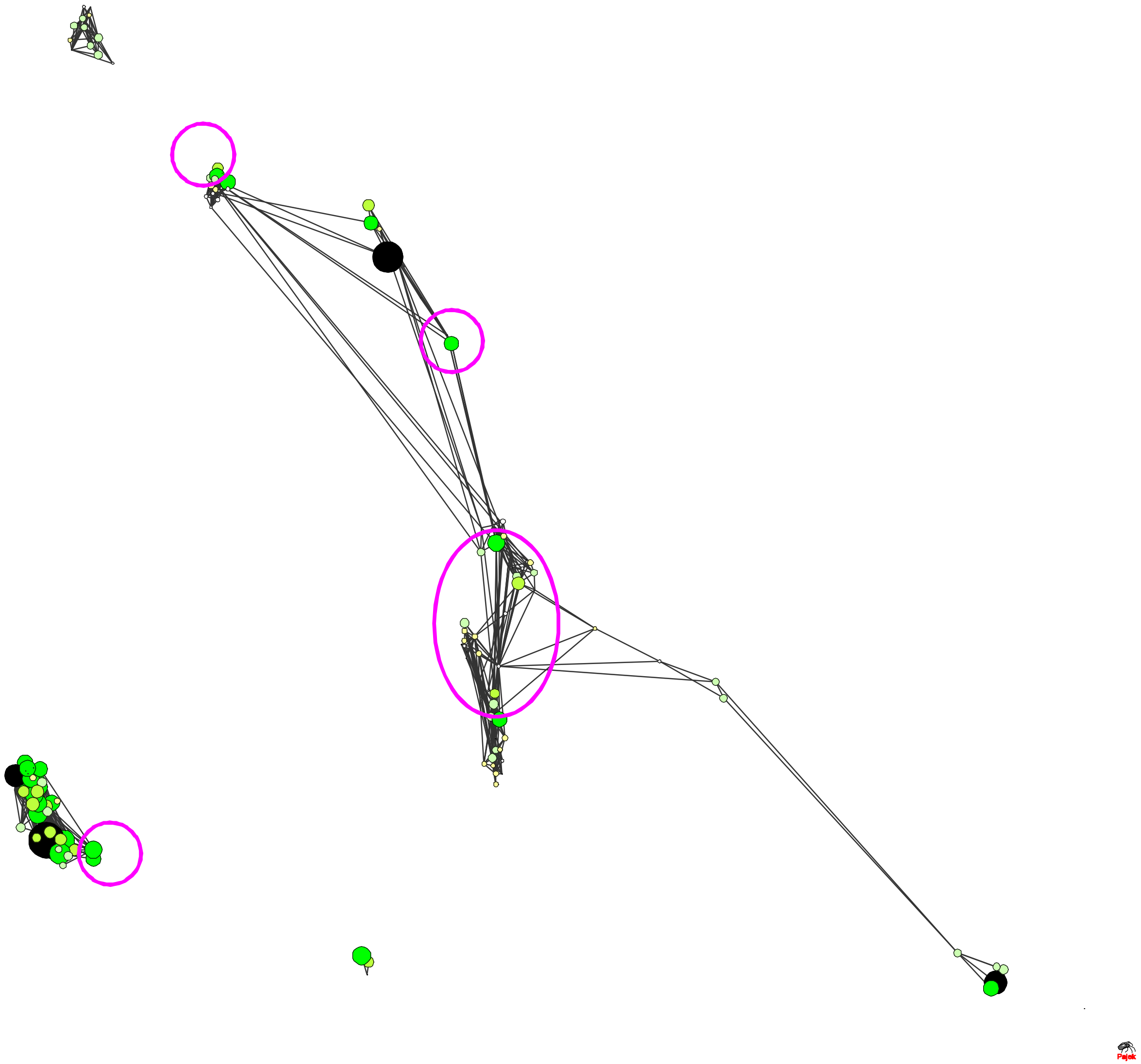
Patent production and impact



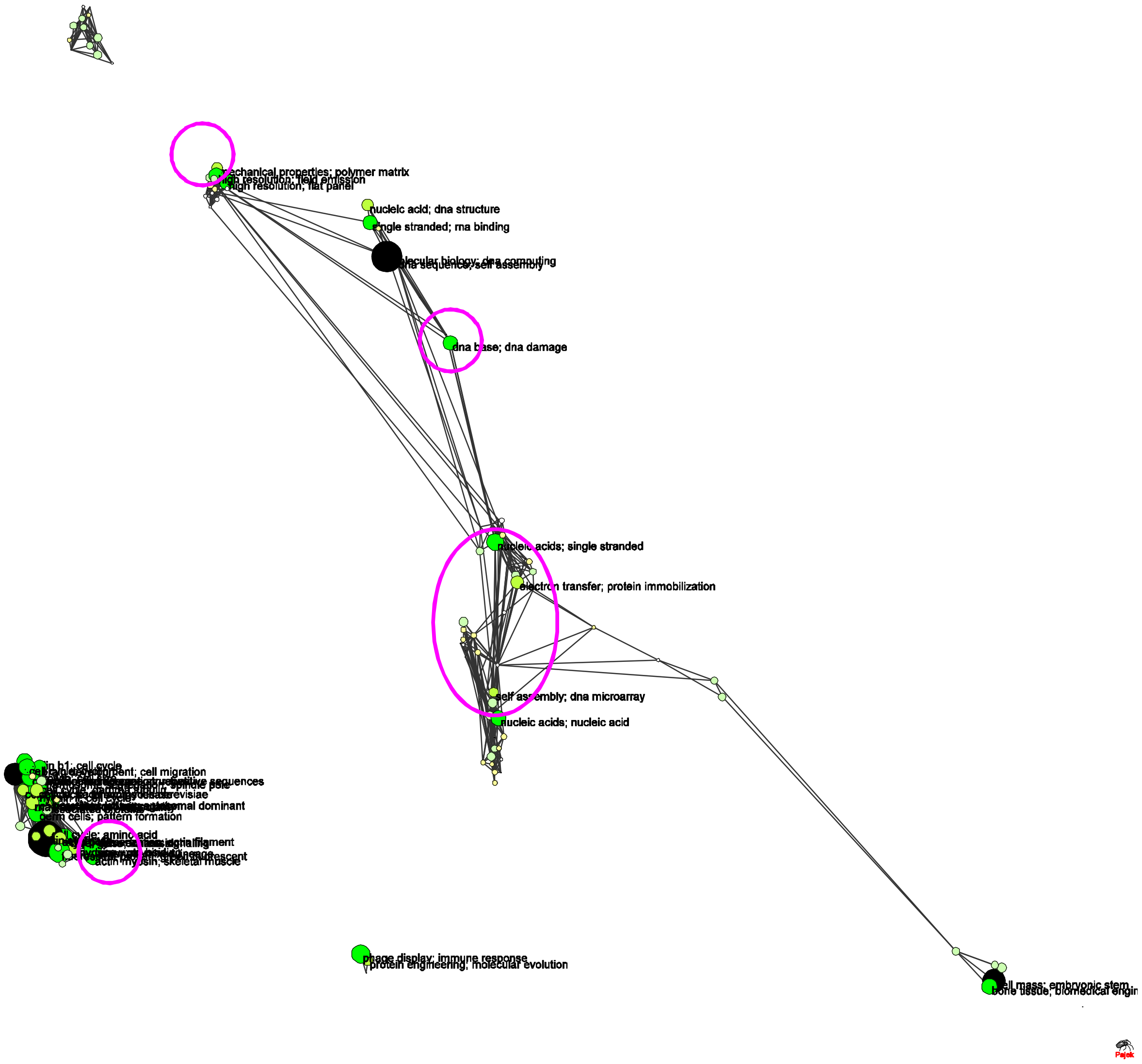
Patent production and impact



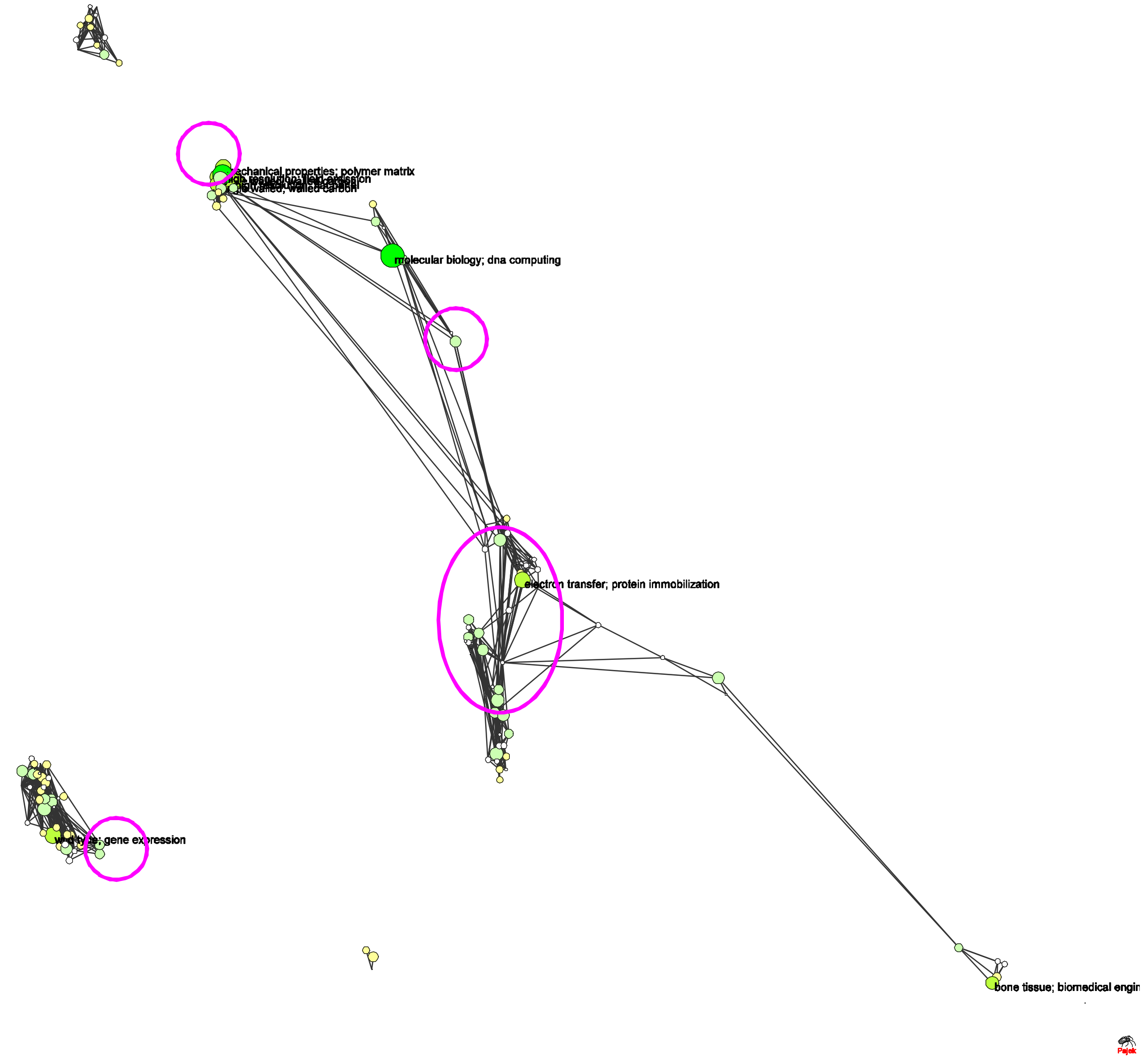
NIH funding



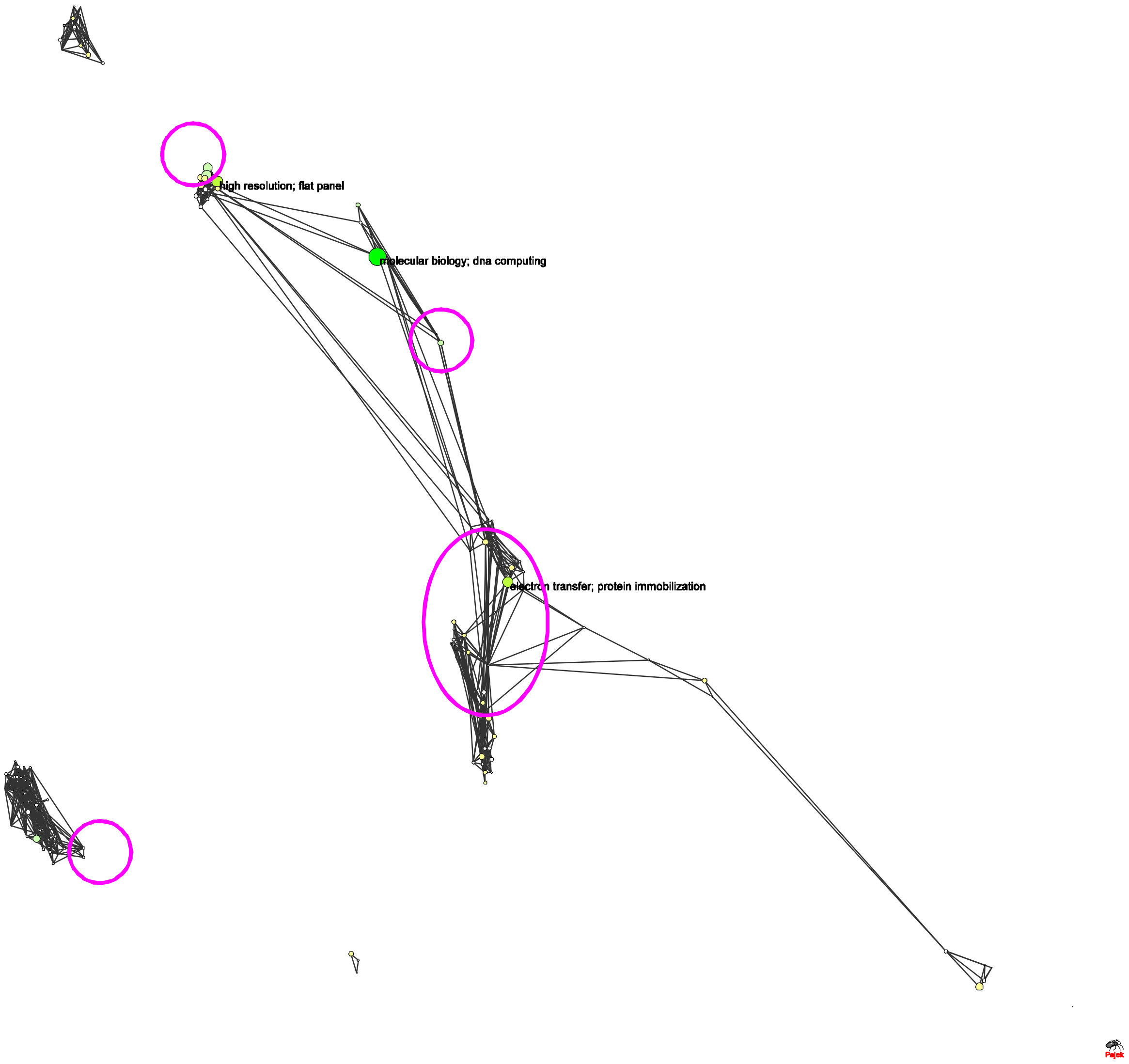
NIH funding


mechanical properties; polymer matrix
high resolution; field emission
high resolution; flat panel
nucleic acid; dna structure
single stranded; rna binding
molecular biology; dna computing
dna sequence; self assembly
dna base; dna damage
nucleic acids; single stranded
electron transfer; protein immobilization
self assembly; dna microarray
nucleic acids; nucleic acid
brain development; cell migration
repetitive sequences
spindle pole
cerevisiae
autosomal dominant
germ cells; pattern formation
cell cycle; amino acid
filament
fluorescent
actin myosin; skeletal muscle
phage display; immune response
protein engineering; molecular evolution
cell mass; embryonic stem
bone tissue; biomedical engin
Pajek

NSF funding


mechanical properties; polymer matrix
high resolution; field emission
single walled; walled carbon
molecular biology; dna computing
electron transfer; protein immobilization
wild type; gene expression
bone tissue; biomedical engin
Pajek

DOE funding


high resolution; flat panel
molecular biology; dna computing
electron transfer; protein immobilization
Pajek

Recap

- Defining the field properly – getting the right data – is critical to getting the best results
- Journal-based searches miss far too much material, and often include material that is not relevant
- Keyword-based searches can be very good
  - Require a great deal of SME interaction and multiple iterations to generate a well-posed query
  - Can still miss material that doesn't use the "right" words
- Mapping all of science (or large chunks) and using our new iterative method for selecting appropriate clusters gives very good results
  - Very good topic focus
  - Includes material that would not be found from keyword searches
  - Clearly shows linkages to other related topics/fields

Recap

- Patents can be linked to science maps
  - They give a retrospective view on the established working paradigms in science that are having a commercial impact
- Grants can be linked to science maps
  - They give a prospective view of which working paradigms are currently well funded
  - Comparison of patent and grant visuals can give us an idea of where publicly funded science will be available to draw upon for commercial activity
- Linking patents and grants isn't limited to our new method, but can be done with keyword-based analyses, making it valuable for exploring commercial opportunity

What if I don’t have the “all of science” data?

- If you have data on hand, use all of what you do have
  - Map your holdings so the results can be used for multiple analyses
  - Detailed method descriptions are available in my publications
    - Email me, and I’ll put them on FTP for you
  - Use the starting point and iterative cluster selection process
- If you have online access, use the keyword-based query model
  - Map the query results using the same process used for the “all of science” maps
  - Keep your resulting datasets and merge them once you have several
- If you have Web of Science access, consider using CitespaceII, freeware by Chaomei Chen, Drexel for mapping
- Patent and grant data are free, and can be linked to your maps using simple database routines
    - Patent data – weekly update XML files at www.uspto.gov
    - Patent data – Google patents – hire a student to scrape it
    - Grant data – RAND RaDiUS database, get a password, most records have unlimited access