# Emerging trends and needs in scientific publishing: Views of a material scientist and chemical engineer

**Arthi Jayaraman**

**Associate Professor**

**Graduate Program Director**

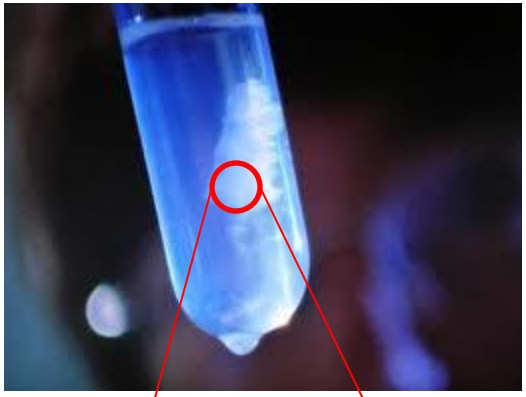
**Dept. of Chemical and Biomolecular Engineering**

**(Joint appointment) Dept. of Materials Science and Engineering**

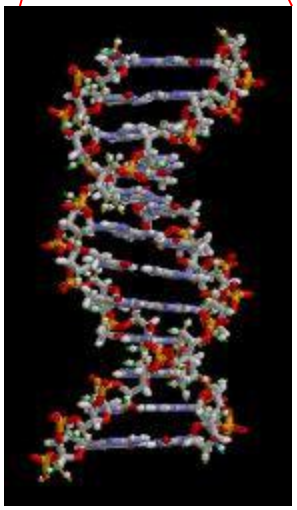
**University of Delaware, Newark**

# Engineering novel materials from the molecular level

## Delivery of Therapeutics

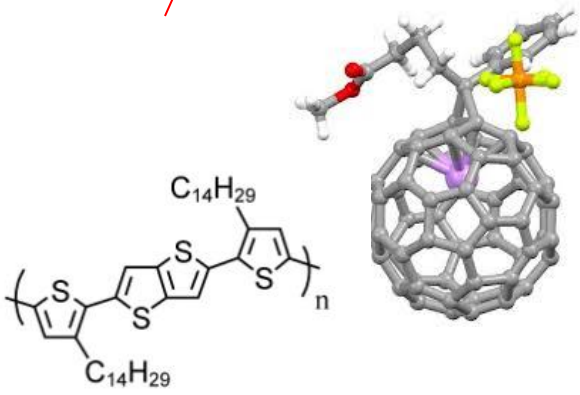


roadwolf.ca

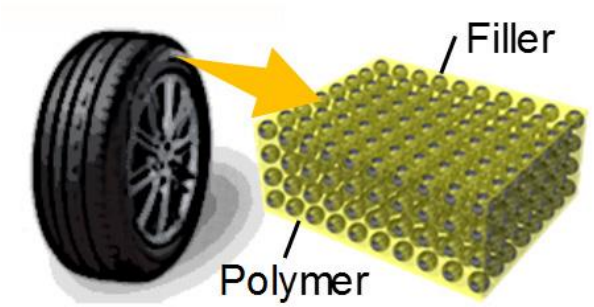


## Solar Cell

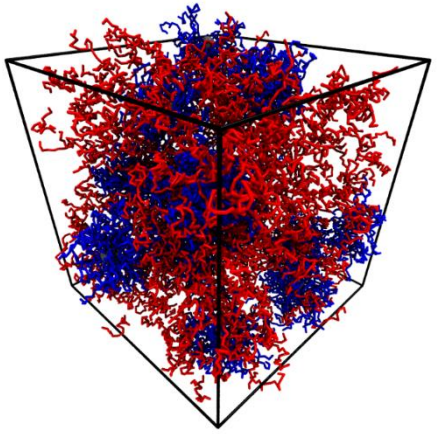
en.wikipedia.org




## Polymer Nanocomposites

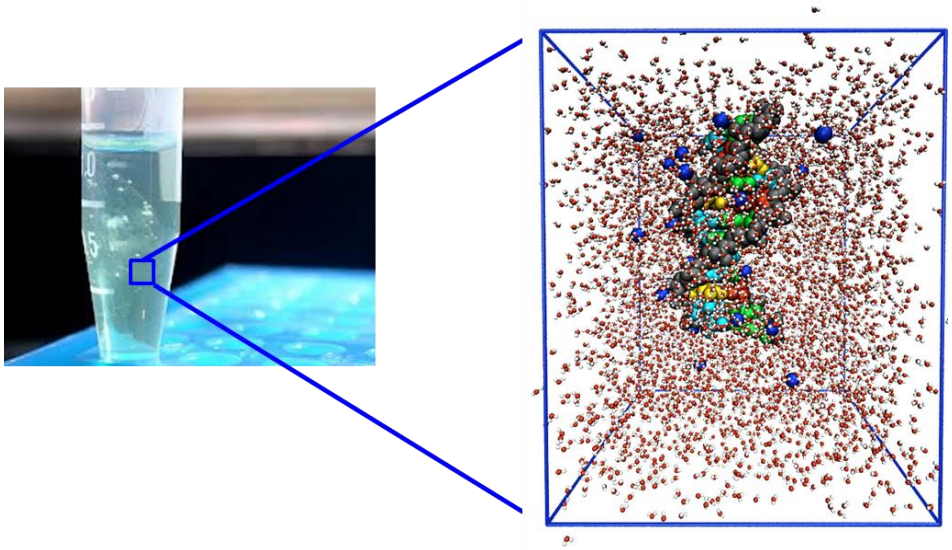



http://www.ifs.kyushu-u.ac.jp/



# The tools we use: Molecular simulations

Provide a microscopic view of the way the molecules move in a variety of chemical/materials/biological systems



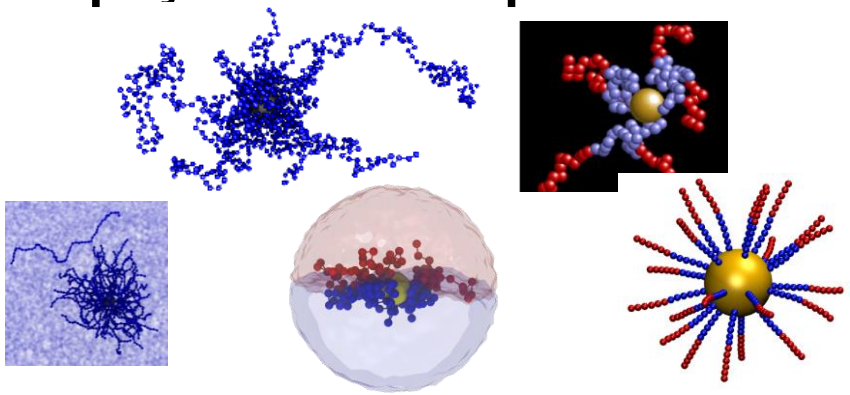
**Molecular simulations**

- **are cheaper, safer and faster than experiments if one wants to scan a large design space**
- can guide experimentalists/synthetic chemists on what to "engineer/design" next

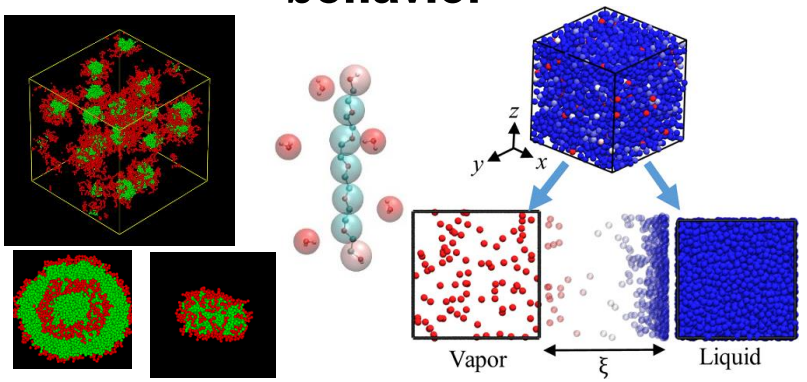
# Computational Studies of Polymers in Jayaraman Group (2008 – present)

## Designing polymers at the molecular level for engineering novel materials

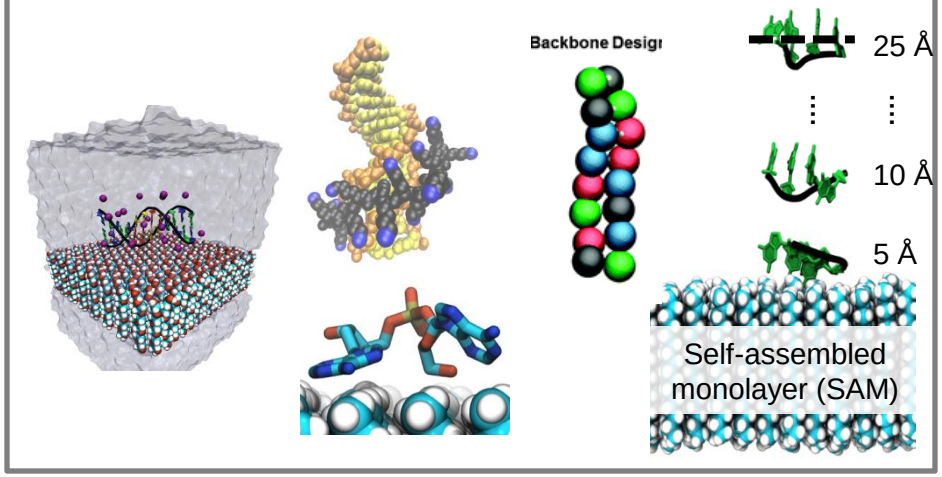
### Functionalized nanoparticles in polymer nanocomposites



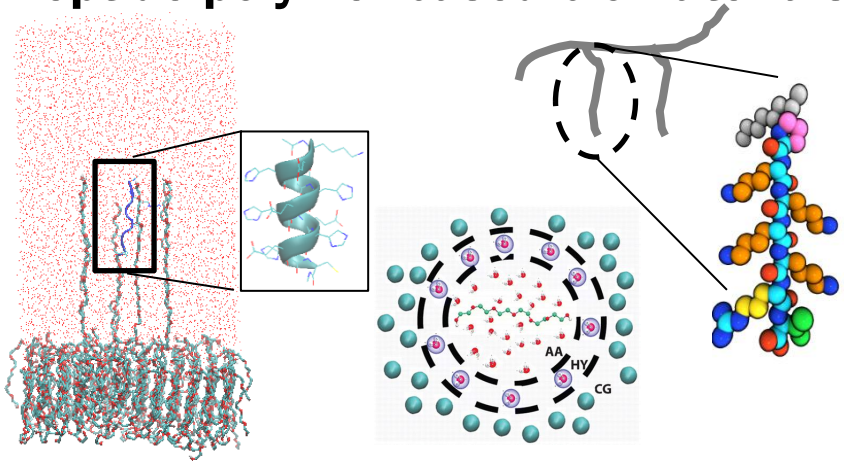
### Solvent effects on polymer behavior



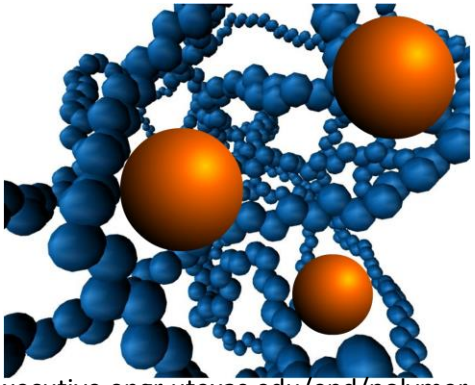

### Nucleic acids based materials




### Peptide-polymer based biomaterials



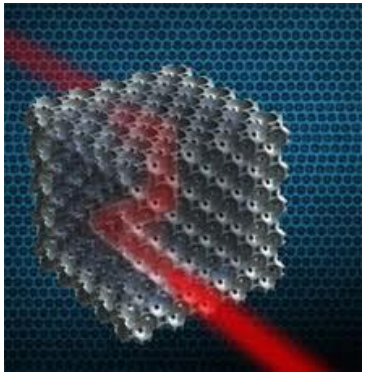
# I. Polymer Nanocomposites



http://executive.engr.utexas.edu/epd/polymer_nano.php

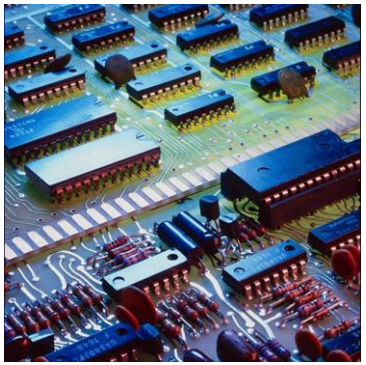
Nanoparticles embedded in polymer matrix

Optics



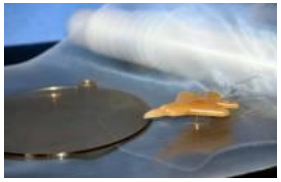
Scienceahead.com

Microelectronics



Chlorineremoval.com

Bottles, films, automotive parts

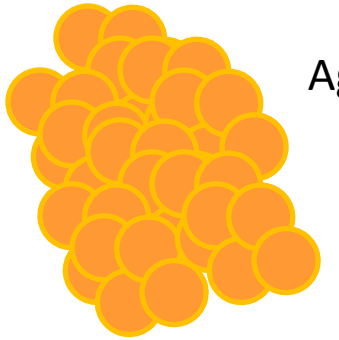




**The ability to tailor the spatial arrangement of nanoparticles in a polymer matrix is critical to applications**

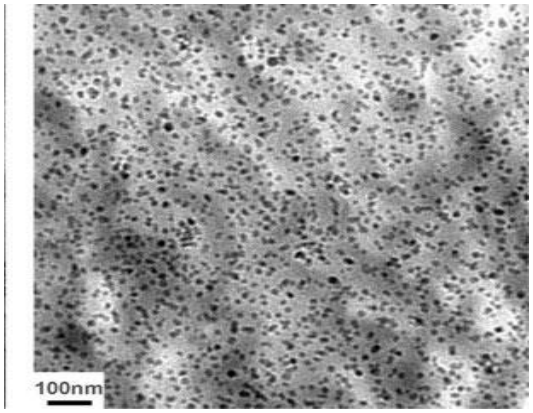
# Need to functionalize nanoparticles

If left unfunctionalized they will aggregate



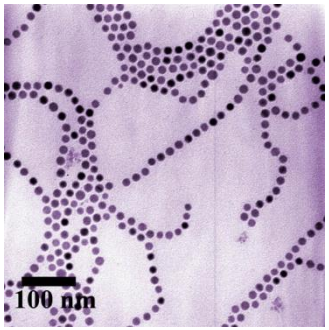
Aggregated

Some applications need nanoparticles to remain **dispersed**




Bates and coworkers, J. Polym. Sci. B: Polym. Phys., 45, 2284 (2007)

Some applications need nanoparticles to be **ordered**

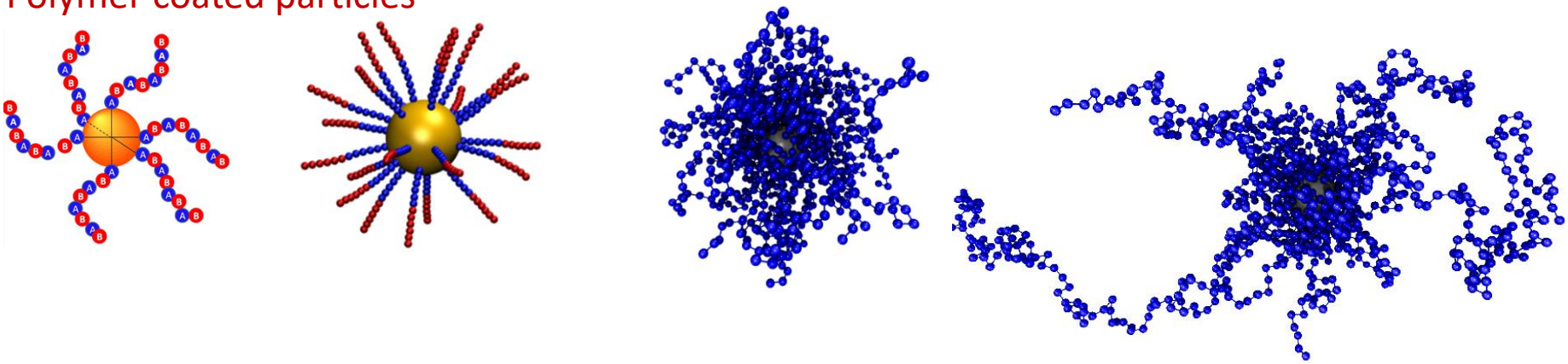



In arrays

Transmission electron micrograph showing chains of cobalt nanoparticles.
Image credit: G. Cheng, A.R. Hight Walker/NIST

# Design rules for polymer functionalization to tailor nanoparticle arrangement

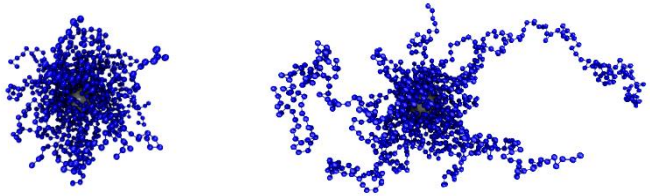
Polymer coated particles



We use theory and simulations to design or “tailor” the right coating/functionalization on the nanoparticle to tune the interactions between nanoparticles, and thus their arrangement in the desired medium

# Examples of Design Rules We Have Found

Increasing graft polymer molecular weight dispersity improves particle dispersion



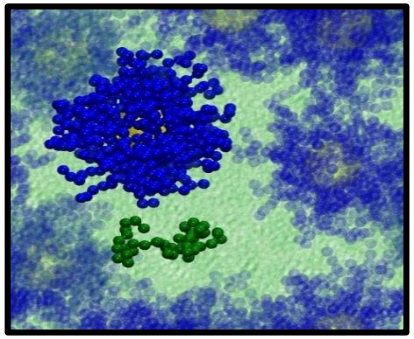
Martin T.B., Dodd P.M., Jayaraman A., *Phys Rev Lett* (2013), 110 (1), 018301

Chemically attractive graft and matrix polymers improve dispersion

Martin T.B. et al. *JACS* (2015) 137 (33), 10624–1063155.

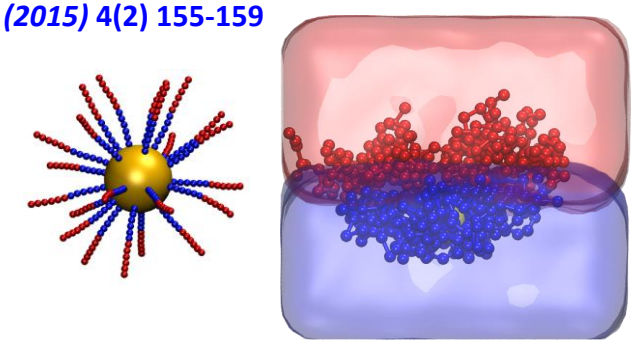
Martin T.B., Jayaraman A., *Macromolecules*, (2016) 49 (24), 9684–9692

*Materials Research Express* (2016) 3, 034001



Block copolymer grafted nanoparticles compatibilize interfaces in homopolymer blends

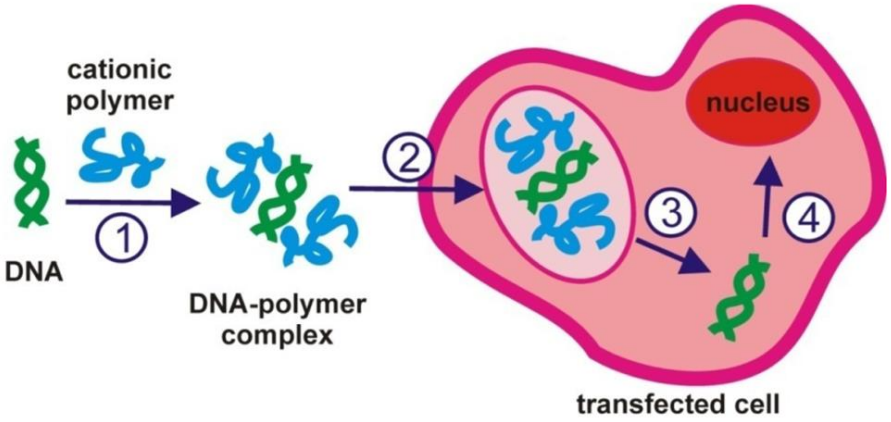
Estridge, C.E.; Jayaraman A. *ACS Macro Letters (2015)* 4(2) 155-159



# II. Polymers for therapeutic DNA delivery

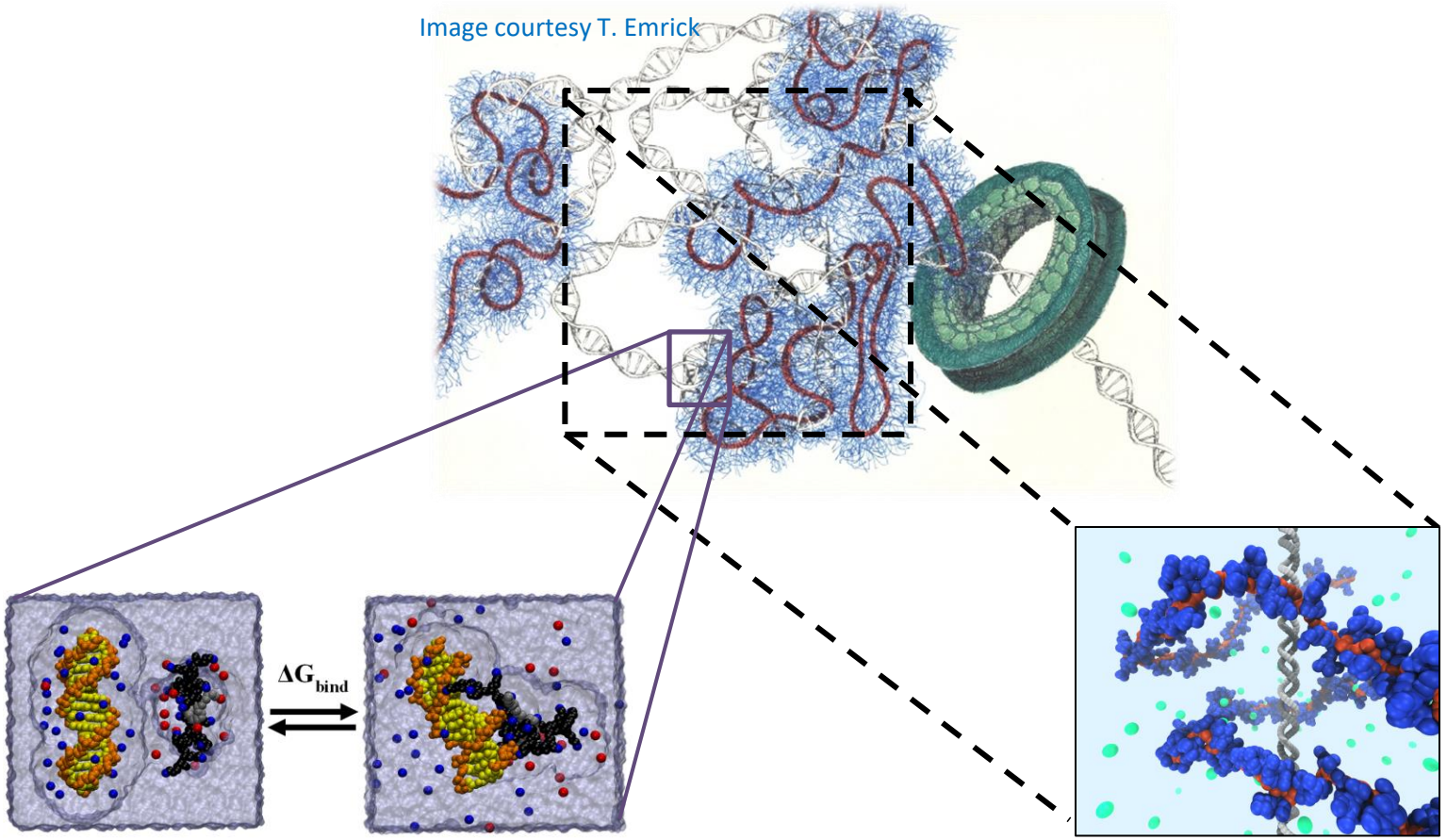
To delivery therapeutic DNA to the body, there is a need for biocompatible polymers that

- avoid side effects of viruses
- have low toxicity,
- protect DNA during transport,
- deliver DNA well




http://www.mdpi.com/2073-4360/3/3/1215/htm

# Multi-scale molecular simulations

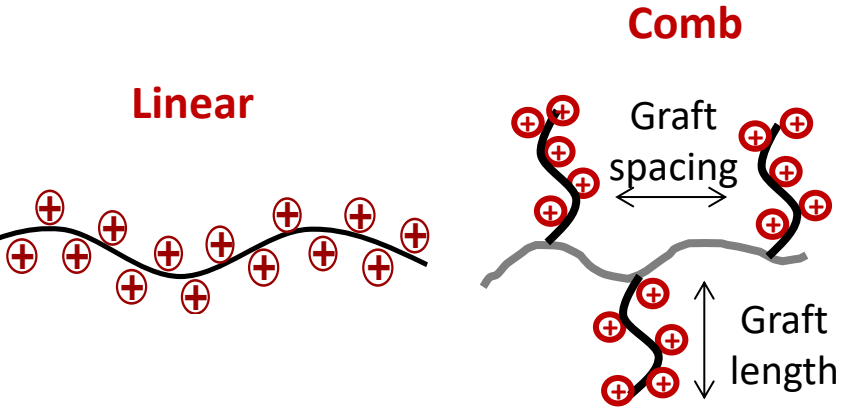


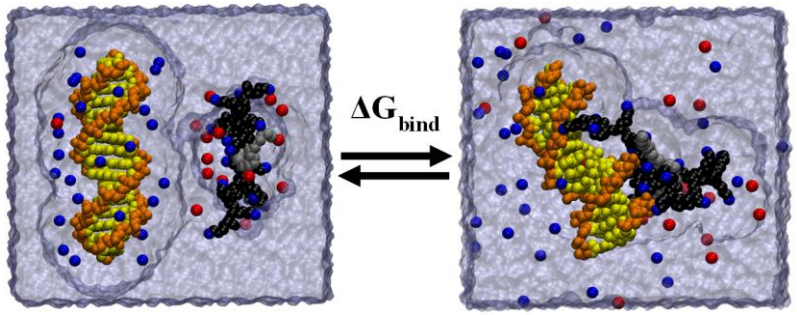

Simulations of polymer-DNA binding at **atomistic** level

Simulations of polymer-DNA binding at a **larger than atomistic** scale

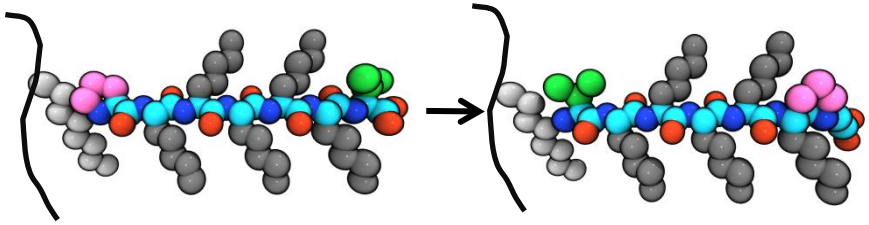
# Linking polymer design to DNA delivery efficacy


**Effect of Varying Polymer Architecture**
**On Polymer DNA Binding Thermodynamics**



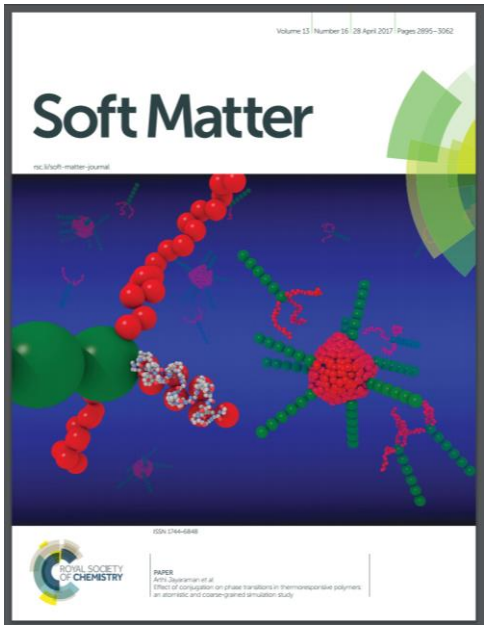

**Effect of Varying Oligopeptide-based Comb-Polymer Chemistry**

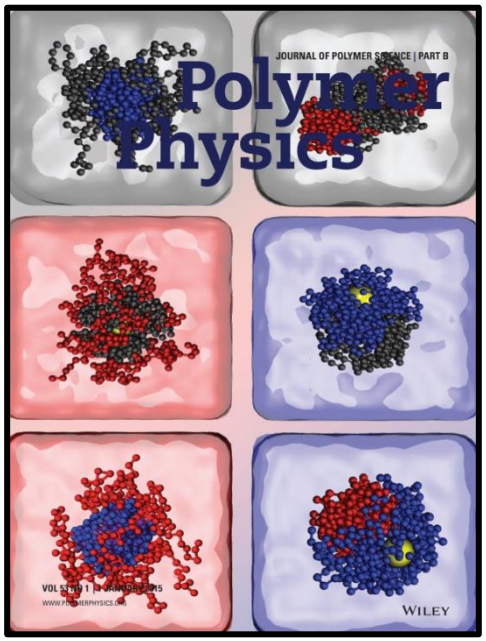


**R. M. Elder and A. Jayaraman, *J. Phys. Chem. B.* (2013)** 117 (40), pp 11988–11999

**R. Elder, T. Emrick, and A. Jayaraman,**
***Biomacromolecules* 12 (11), 3870 (2011)**

# Journals we publish in




**American Chemical Society Journals**
Macromolecules
Biomacromolecules
ACS Macro Letters
Journal of Physical Chemistry B
Journal of American Chemical Society (JACS)
Journal of Chemical Theory and Computation

**Wiley Journals**
Journal of Polymer Science part B: Polymer Physics

**Royal Society of Chemistry Journals**
Soft Matter
Molecular Systems Design and Engineering

**American Institute of Physics Journals**
Physical Review Letters
Journal of Chemical Physics

**Taylor and Francis Journals**
Molecular Simulation

# Emerging trends and needs in publishing for computational materials science

## 1. To enhance reproducibility all journals should require raw data from authors

Taken from http://journals.plos.org/plosone

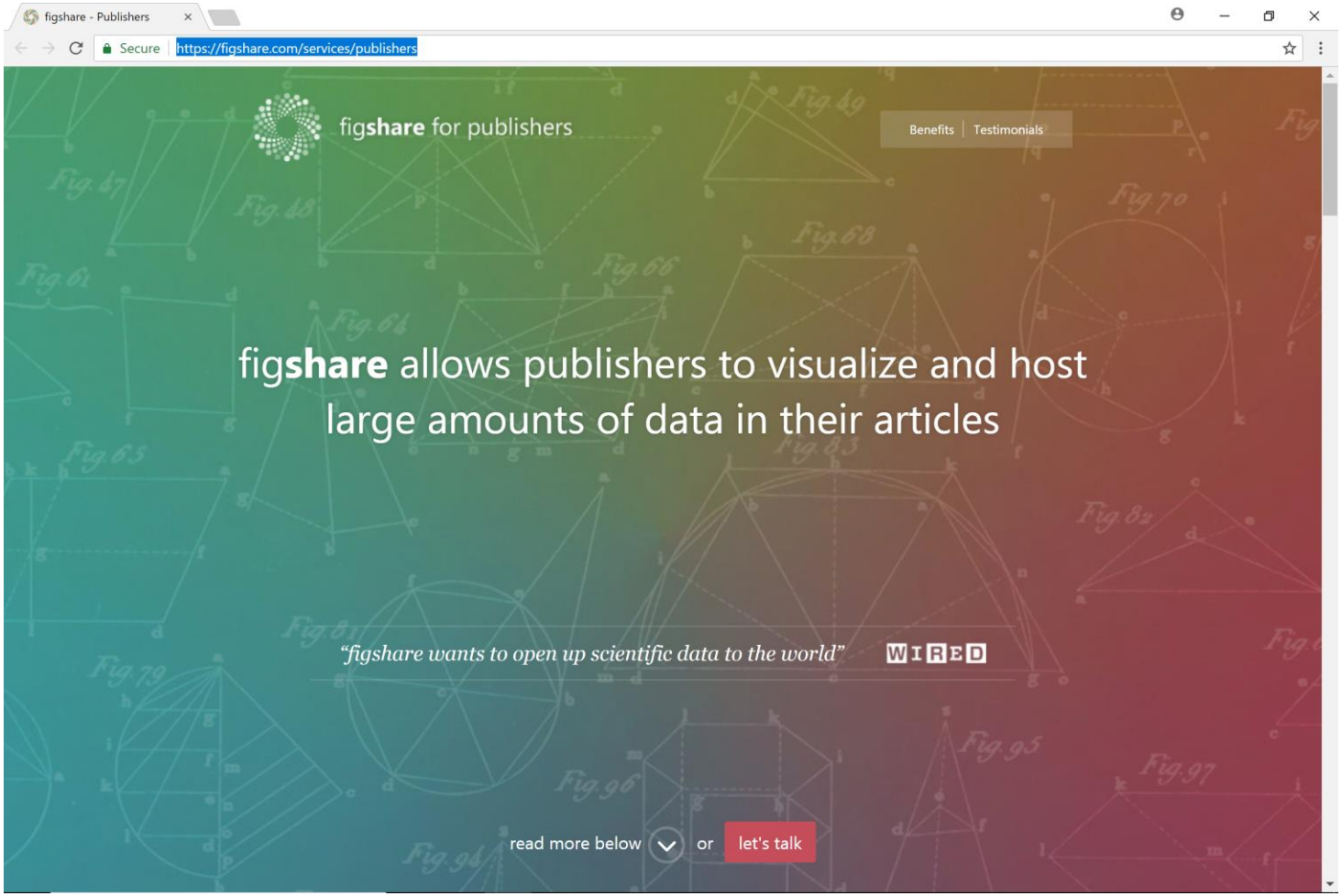
*"All data and related metadata underlying the findings reported in a submitted manuscript should be deposited in an **appropriate public repository**, unless already provided as part of the submitted article.*

**Don't just encourage data sharing, enforce data sharing.**

## How about the journals hosting this public data?

- Will enforce proper citation of the raw data
- Will allow publication of "negative" results
- Will enable searching of raw data for specific topics
- Will enable data mining and machine learning

# Emerging trends and needs in publishing for computational materials science



# Emerging trends and needs in publishing for computational materials science

## 2. Need to enforce submission of analyses codes and algorithms

Taken from https://www.nature.com/news/code-share-1.16232

## Code share

*Papers in Nature journals should make computer code accessible where possible.*

A theme in *Nature*'s ongoing campaign for the replicability and reproducibility of our research papers is that key components of publications should be available to peers who wish to validate the techniques and results.

A core element of many papers is the computer code used by authors in models, simulations and data analysis. In an ideal world, this code would always be transportable and easily used by others. In such a world, our editorial policy would be to insist on sharing to allow free use, as we already do (as far as is practicable) with data and research materials. Unfortunately, such an ideal is not easy to attain owing to the amount of extra funding and effort it would require to render some major pieces of code shareable. Nevertheless, we at *Nature* and the Nature research journals want to encourage as much sharing as possible.

Climate modellers have made some strides in this regard. The journal *Geoscientific Model Development* has a good example of such a policy (see go.nature.com/jv8g1w), and an article in *Nature Geoscience* discusses some of the opportunities presented by code sharing, as well as the obstacles (S. M. Easterbrook *Nature Geosci.* 7, 779–781; 2014).

As a leading example of transparency policies in other disciplines, the data journal *GigaScience* requires code used in its papers to be available, and hosts it in a way that allows others to analyse the data in publications. One point made by Easterbrook is that even if the code is shared, others might often make little or no use of it, but on some occasions the take-up will be large.

*Nature* and the Nature journals have decided that, given the diversity of practices in the disciplines we cover, we cannot insist on sharing computer code in all cases. But we can go further than we have in the past, by at least indicating when code is available. Accordingly, our policy now mandates that when code is central to reaching a paper's conclusions, we require a statement describing whether that code is available and setting out any restrictions on accessibility. Editors will insist on availability where they consider it appropriate: any practical issues preventing code sharing will be evaluated by the editors, who reserve the right to decline a paper if important code is unavailable. Moreover, we will provide a dedicated section in articles in which any information on computer code can be placed. And we will work with individual communities to put together best-practice guidelines and possibly more-detailed rules.

For full details, see our guide for authors at go.nature.com/o5ykhe. For an archive of our content and initiatives concerning reproducibility, see http://www.nature.com/nature/focus/reproducibility. ■

NATURE.COM
To comment online, click on Editorials at: go.nature.com/xhunqv

536 | NATURE | VOL 514 | 30 OCTOBER 2014



*"A core element of many papers is the computer code used by authors in models, simulations and data analysis. In an ideal world, this code would always be transportable and easily used by others. In such a world, our editorial policy would be to insist on sharing to allow free use, as we already do (as far as is practicable) with data and research materials. Unfortunately, such an ideal is not easy to attain owing to the amount of extra funding and effort it would require to render some major pieces of code shareable."*

# Emerging trends and needs in publishing for computational materials science

## 3. It is time to consider open review process or a hybrid open online review-blind offline review

***Some issues with the single-blind peer-review***

https://doi.org/10.3389/fnins.2015.00169

1. Bias against specific categories of paper.
2. Social and cognitive biases.
3. Unreliable reviewer assessment
4. Inability to detect errors and fraud.
5. Lack of transparency—unethical practices

**What is a hybrid review**:

- an open and informal review on the internet
- after the above/simultaneously a formal (blind review) process
- Via this formal/informal review process, the editorial team makes the final decision
- For example adopted by Atmospheric Chemistry and Physics (ACP)

# Acknowledgements

**Financial Support**

- DOE Early Career Award (2010-2015)
- DOE BES Materials Chemistry
- NSF DMR, CBET, DMREF
- NERSC and XSEDE Supercomputing
- UDelaware Farber computing

**Current Group Members**

- Thomas Gartner, 4th year grad student
- Michiel Wessels, 2nd year grad student
- Arjita Kulshesthra, 1st year grad student
- Phillip Taylor, 1st year grad student
- Kevin Modica, UG Junior
- Daniel Intriago, UG Junior
- Dr. Ivan Lyubimov
- Dr. Daniel Beltran
- Dr. Prhashanna Ammu

**Past Group members (current position)**

- Josh Condon MS 2017 (Capital One)
- Tyler Martin PhD 2016 (NIST)
- Dr. Ahmad Ghobadi (P&G)
- Hilary Marsh PhD 2015 (Ch2M)
- Carla Estridge, PhD 2015 (Boeing)
- Robert Elder PhD 2014 (ARL)
- Arezou Seifpour, PhD 2013 (Intel)
- Dr. Francesca Stanzione
- Dr. Nitish Nair (Shell)
- Dr. Eric Jankowski (Boise State)
- Dr. Donsgsheng Zhang (UT Dallas)
- Dr. Steve Dahl (BP)
- Dr. Nate Wentzel (Milligan)
- Paul Dodd, Senior thesis (Michigan)
- Brandon Lin, Senior thesis (BP)
- *+ other masters students and undergraduates*