Electrostatic shape control of a charged molecular membrane from ribbon to scroll

Scientific Achievement
Through experimental and theoretical studies, molecular reordering driven by variations in electrostatic screening length is shown to induce micrometer scale structural changes in crystalline membranes of charged, chiral molecules.

Significance and Impact
Our study suggests that these structural changes should be general to charged bilayers possessing a spontaneous curvature, and applicable to many applications, including drug delivery and photocatalytic production of hydrogen.

Research Details
– With the addition of NaCl, high aspect ratio C_{16}K_{1} ribbons formed in zero salt conditions transform to isotropic sheets, prior to rolling up to form cochleates.
– A simplified model demonstrates that the ribbon to sheet transformation is a first-order transition induced by the reduction in the range of electrostatic interactions.
– Theoretical models show that rolling of membranes into cochleates is the combined effect of molecular chirality and tilt.

Changrui Gao, et al., PNAS 116, 22030-22036 (2019); DOI: 10.1073/pnas.1913632116

Figure. (A) The geometry of the cochleates. D is the interbilayer separation. Arrows represent the projection of the tilt vector in the local tangent plane. (B) Theoretical prediction showing a roughly linear relationship between interbilayer spacing D and c−1/2, where c is NaCl molar concentration.

Work was performed at Northwestern University
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Title
Attention grabbing and accessible but not exaggerated

Text
All text should be short and to the point – minimize words and stress significance to society
- **Scientific Achievement** – 50 words or less
- **Significance and Impact** – 50 words or less
  Importance, relevance, or intriguing component of the finding to the field
- **Research Involved** – Address the research approach in 2-4 bullet points
  Give a ~175 word detailed explanation plus additional description of figure if needed in the PowerPoint Notes section

Citation
Full citation with all authors’ names is preferable
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Figures
Visually compelling figure(s) to explain the research
Include legends and descriptive caption
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Institutional logo(s)
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Indicate institution where research was performed (if possible); EFRC and Hub research should include those logos as well

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**New Mechanism for Design of Radiation Damage Resistant Materials**

**Scientific Achievement**
Computer simulations explain why some nanostructured materials exhibit increased tolerance to radiation damage

**Significance and Impact**
Mechanism suggests new routes to self-healing of radiation damaged materials, an important advance for nuclear energy

**Research Details**
- Radiation knocks atoms out of their preferred sites creating interstitials and leaving behind vacancies
- Previously, it was thought that once interstitials moved to grain boundaries they were trapped and unavailable to recombine with vacancies
- Temperature-accelerated dynamics simulations showed grain-boundary interstitials can be re-emitted to combine with vacancies at a rate faster than other recombination mechanisms
- Grain boundaries in designed nanostructured materials could slow down damage accumulation

*Schematic of recombination mechanism:* After irradiation interstitials migrate to the grain boundary leaving vacancies behind. Some interstitials escape the grain boundary to recombine with the vacancies several atomic distances away. The few vacancies left behind typically join to form a larger defect.


Work was performed at Los Alamos National Laboratory
Scientific Achievement

New calculations demonstrate that LED “droop” is dominated by multi-particle interactions. Droop occurs when increasing energy input does not produce proportionally more light.

Significance and Impact

Understanding “droop” may result in cheaper, more efficient LEDs; LEDs are more energy efficient, smaller, and longer-lived than incandescent lamps or fluorescent lighting.

Research Details

– Atomistic first-principles calculations indicated that increasing amounts of indium in Indium Gallium Nitride (InGaN) green LEDs caused a decrease in light intensity.
– Computational data was confirmed by experimental spectroscopic evidence which showed electron-phonon coupling and alloy scattering (breaking of symmetry due to the insertion of Indium) to be important processes.


Work was performed at University of California – Santa Barbara.
New Catalyst Speeds Conversion of Electricity to Hydrogen Fuel

**Scientific Achievement**
A newly synthesized nickel complex speeds the production of hydrogen ten times faster than a natural hydrogenase enzyme at room temperature.

**Significance and Impact**
Opens a new research path to develop long-lived catalysts using inexpensive, earth-abundant metals to convert electrical energy to chemical energy.

**Research Details**
- In this process, water molecules are split to produce hydrogen and oxygen. Hydrogen can be used as a fuel.
- Using the natural hydrogenase enzyme as a model, a synthetic catalyst using nickel was developed. The metal atom gets its reactive properties from the groups of atoms containing phosphorous and nitrogen that surround it.
- By splitting water, hydrogen gas is formed by combining the H⁺ on the nitrogen with the H⁻ on the nickel center.
- Adding an acid or water increased the rate of hydrogen produced from the newly-designed synthetic catalyst.

Purple Bacteria Develops Its Own Form of “Sunscreen”

Scientific Achievement
Determined that specific pigments in the light harvesting complex found in photosynthetic bacteria act primarily to protect the cell from damage by excess sunlight

Significance and Impact
Provides insights on how to minimize deleterious effects from over exposure to sunlight in the design of man-made systems to gather and use the sun’s energy

Research Details
– In photosynthetic organisms, supplementary pigments called carotenoids capture wavelengths of light that the major pigments can not efficiently harvest
– However, steady-state absorption and fluorescence spectra showed that carotenoids in the photosynthetic bacterium Thermoctomatium tepidum play a negligible role in energy capture and transfer
– Instead, the composition and structure of the carotenoids have been optimized to protect the light harvesting complex from sun damage

The orange ring surrounding Grand Prismatic Spring, Yellowstone National Park, is due to carotenoid molecules, produced by huge mats of algae and bacteria (Photo from http://en.wikipedia.org/wiki/Carotenoid)

E D. M. Niedzwiedzi et al. Photosynthesis Research 2011, 107, 177-186

Work was performed at Washington University in St. Louis

EFRC: Photosynthetic Antenna Research Center (PARC) at Washington University in St. Louis