New Mexico Highlands University
Ohio State University

Light Matter Interactions: Theory and Applications (I)
Partnership between NMHU and OSU in Electronic, Optical and Magnetic Materials (II)

Big Thanks to …

Melissa Hines

Cornell MRSEC

- Chris Hammel
- Ezekiel Johnston-Halperin
- Roland Kawakami
- Jessica Winter
- Andrew Heckler
- Rolando Aguilar

OSU MRSEC

GA Tech

Seth Marder

Sreve Barlow

Viaceslav Coropceanu

NMHU

Carlos Ordonez

Raul Castaneda

Qiang Wei

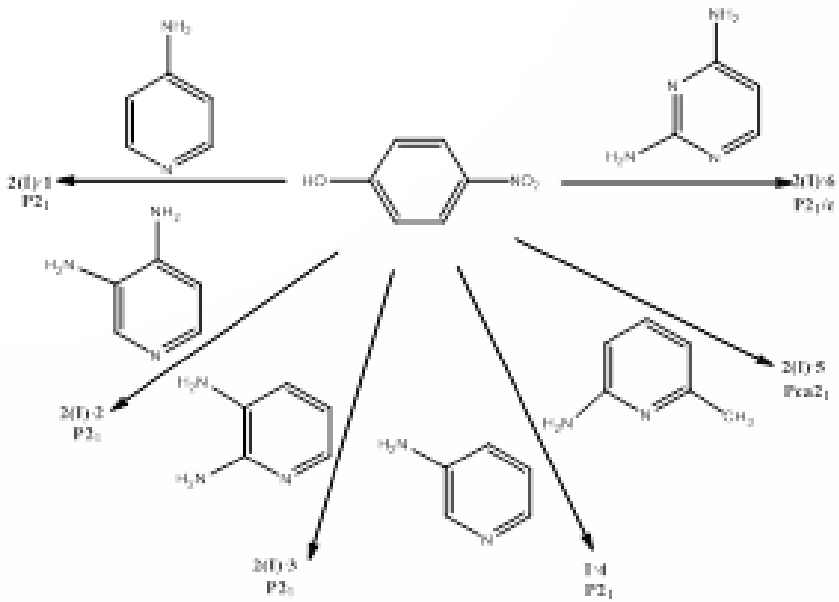
Gil Gallegos

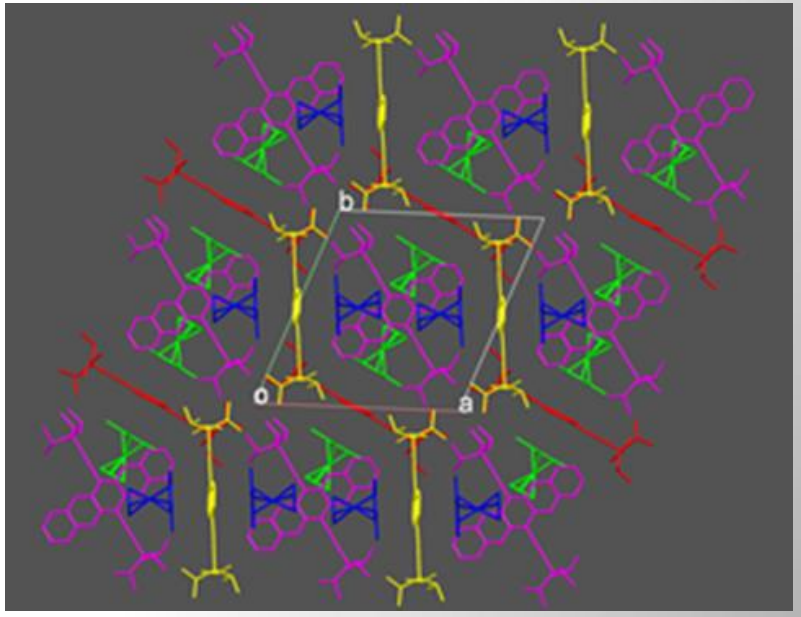
Jiao Chen

Goals of NMHU PREM (I)

- Thrust 1. Design and spectroscopic characterization of two-photon absorbing materials for photodynamic applications.
- Thrust 2. Studies of non-linear optical, electrooptical materials and p- and n-dopants for organic electronics.
- Thrust 3. The synthesis of new electron-transport materials based on naphthalene diimides and derivatives of pyrene and tetrahydropyrene.

Success stories from PREM (I)

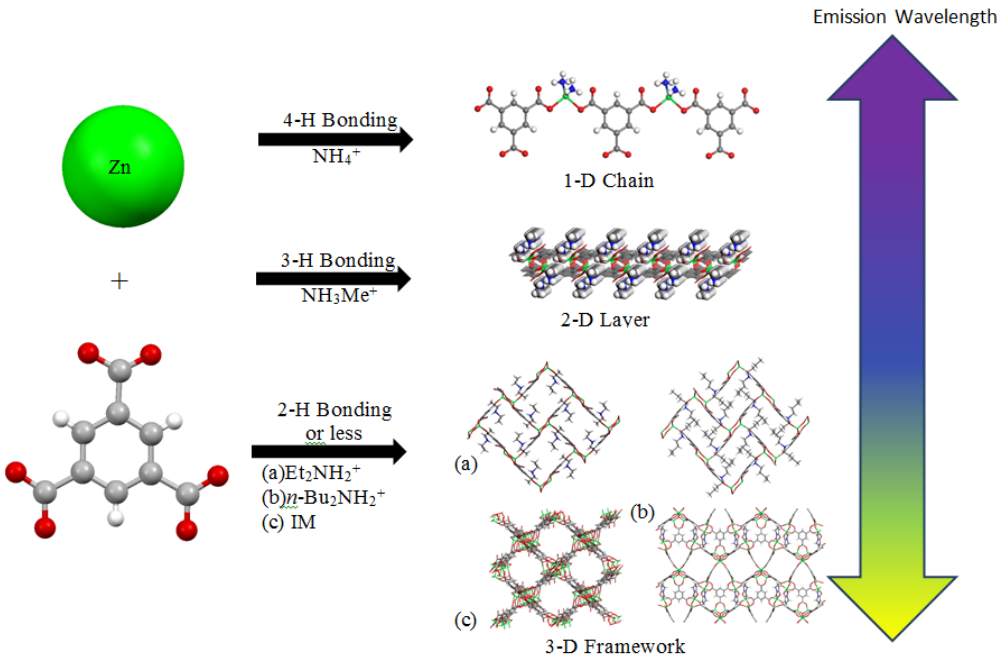


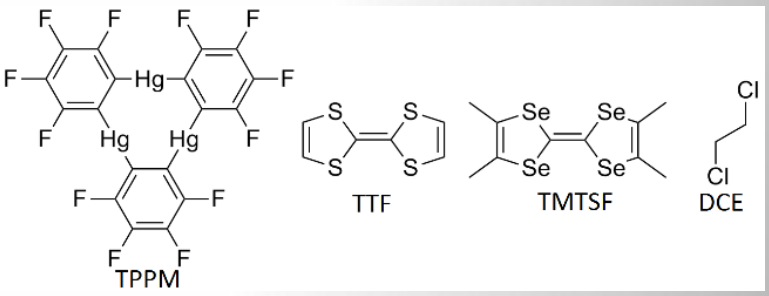


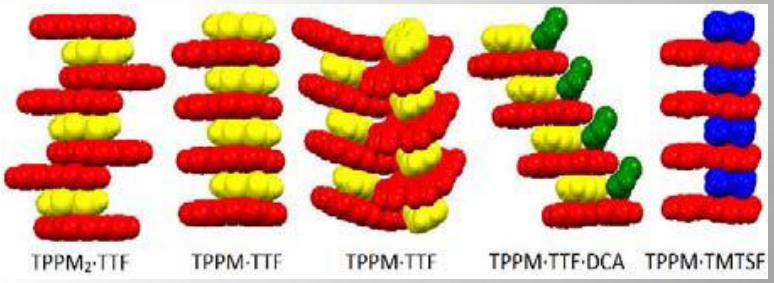
Components, ratio and space groups for p-nitrophenol and aminopyridines adducts – example of acentric co-crystals buit of two non-chiral coformers

Crystal structure of 6,13-Bis(Tri-(isopropyl)-silylethynyl)pentacene (yellow and magenta) doped with RhCpCp* (green and blue) – material for organic field field-effect transistors

Success stories from PREM (I)







Dependence between H-bonding pattern of ligands, dimensionality of synthesized Frameworks and their emission spectra

Structural formulas of donor and acceptor coformers that formed stacked charge transfer materials

List of Participants

Participant	**Affiliation**	**Primary role(s)**
Tatiana **Timofeeva**	Professor, Biology & Chemistry, NMHU	Director, PI – Thrust 1,2
Michael **Petronis**	Associate Prof., Natural Resources, NMHU	Co-PI, Thrust 1,2
Quiang **Wei**	Research Prof., Biology & Chemistry, NMHU	Co-PI, Thrust 2
Jennifer **Lindline**	Professor, Natural Resources, NMHU	Co-PI, Thrust 2
Jiao **Chen**	Assistant Prof., Biology & Chemistry, NMHU	Co-PI, Thrust 3
Gil **Gallegos**	Associate Prof., Engineering & Computer Science, NMHU	Co-PI, Thrust 3
Edward **Martinez**	Associate Prof., Natural Resources, NMHU	Co-PI, Education/Diversity Director
P. Chris **Hammel**	Professor, Physics, OSU	Co-PI, Thrust 1,2
Ezekiel **Johnston-Halperin**	Associate Prof., Physics, OSU	Co-PI, Thrust 1,2
Roland **Kawakami**	Professor, Department of Physics, OSU	Co-PI, Thrust 3
Jessica **Winter**	Associate Prof., Chemical and Biomolecular Engineering	Co-PI, Thrust 3
Andrew F. **Heckler**	Associate Prof., Physics, OSU	Co-PI, Education
Rolando Valdes **Aguilar**	Assistant Prof., Physics, OSU	Co-PI, Education

Goals of NMHU PREM (II)

- Thrust 1. Crystal engineering of materials for electronic, photonic, and magnetic applications.

  (GA Tech, OSU, ITMO)
- Thrust 2. Metal-organic frameworks/aerogels with engineered structure and properties

  (OSU, Argonne NL)
- Thrust 3. Nanomaterials for medicinal applications and nanoparticle-modified graphene metamaterials.

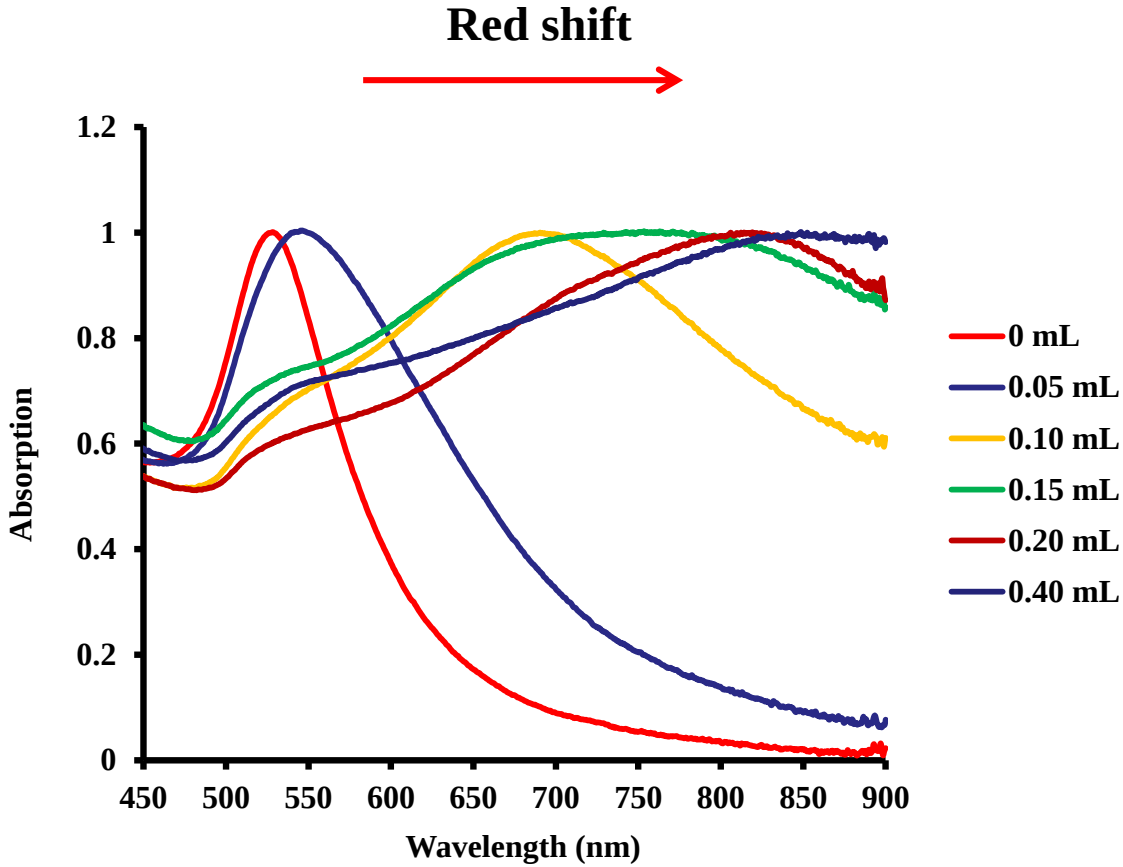
  (OSU)

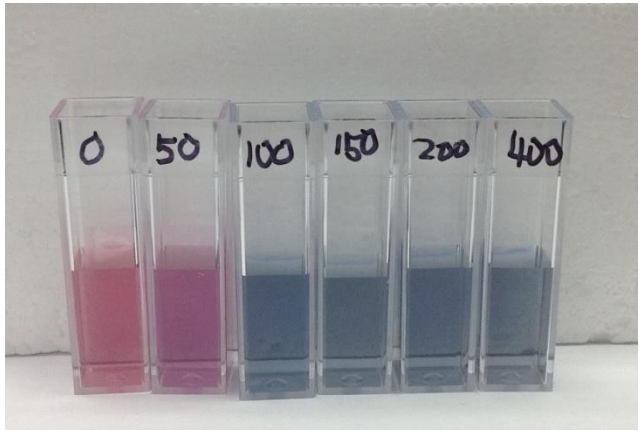
PREM Visitors

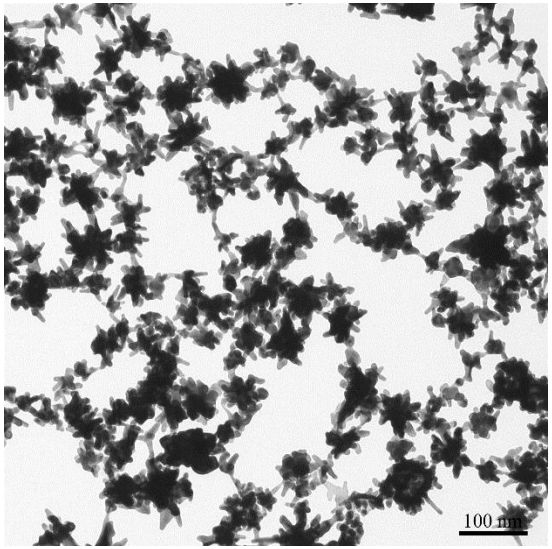
- Dr. Steve Barlow, GA Tech, “Dimeric n-dopants for organic electronics: controlling the thermodynamics and kinetics of strong reducing agents”
- Dr. Javier Read De Alaniz, CA Nanosystem Institute , U Santa Barbara, MRSEC “Developing new transformation for organic synthesis and materials science”
- Dr. Ezekiel Jonstron-Halperin, OSU MRSEC “Organic spintronics: using organic based magnets for flexible low-cost, low-power electronics

Ezekiel Johnston-Halperin visit to NMHU

Development of a novel synthetic method for gold nanostars

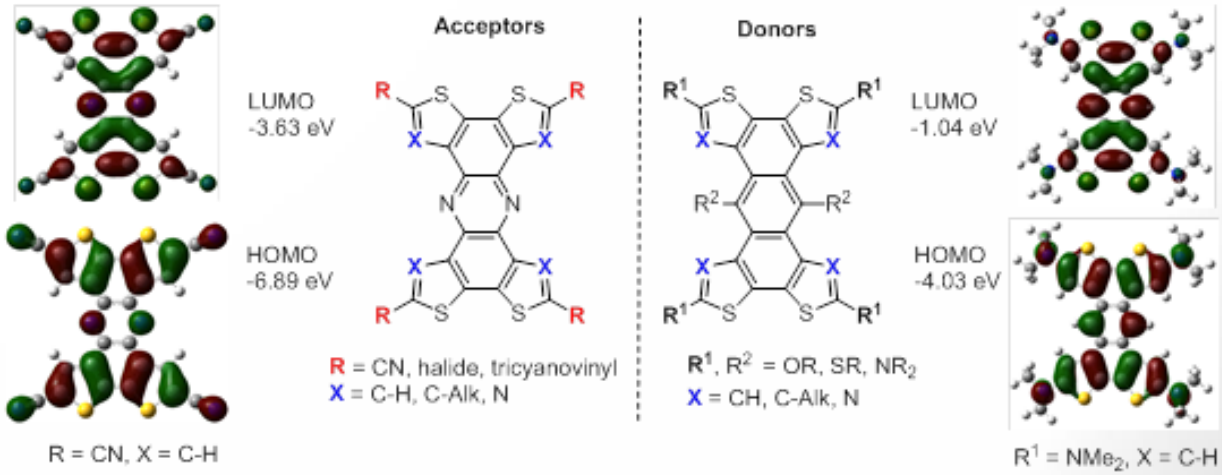






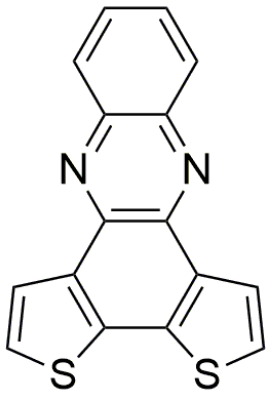
UV-vis absorption spectra of the synthesized Au nanostars. The amount of adding $AgNO_3$ changed from 0, 0.05, 0.10, 0.15, 0.20, to 0.40 mL, respectively. The shape of gold nanomaterials and UV absorption can be easily tuned by different amounts of $AgNO_3$.

Crystal engineering of materials

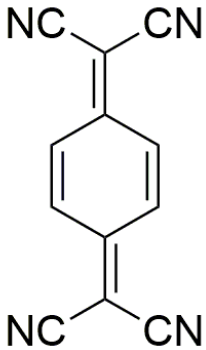


Potential phenazine-based acceptors and anthracene-based donors with similar geometries (frontier molecular orbital energies and wave function illustrations for one example of donor and acceptor molecules are shown, as determined at the B3LYP/6-311G** level of theory).

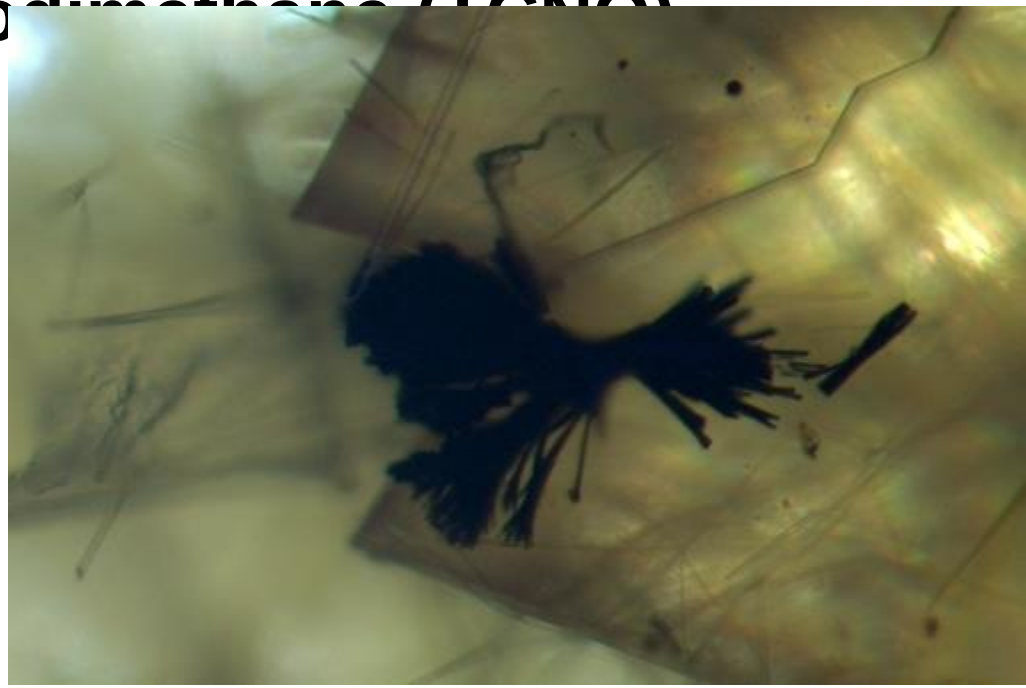
Mixed-Stack Co-Crystals of Dithieno[3,2-*a*:2',3'-*c*]phenazine (DTPhz) and Tetracyanoquinodimethane (TCNQ)



DTPhz



TCNQ

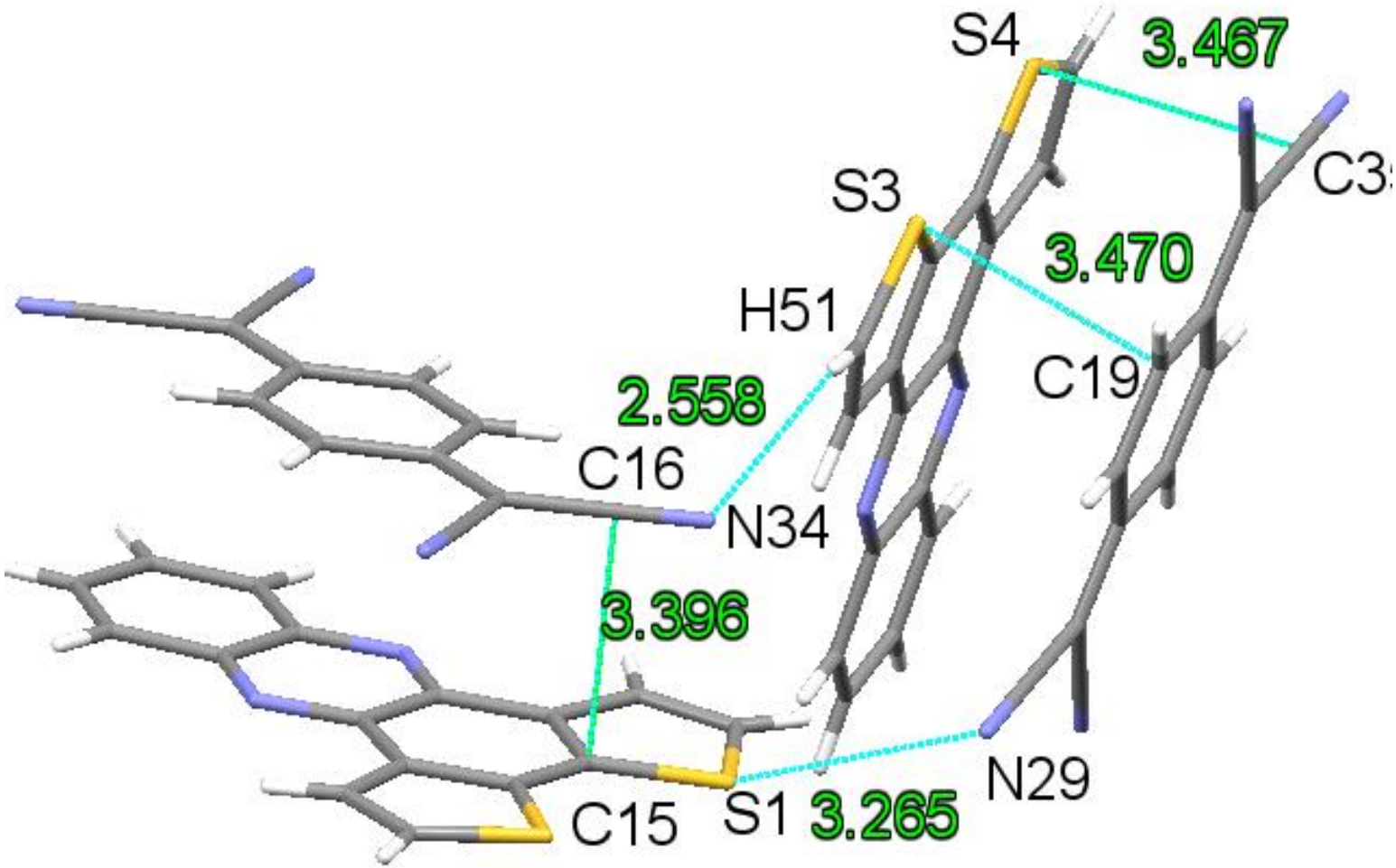


$E^{0/+}$ = +1.08 V[1] $E^{0/-}$ = -0.3 V

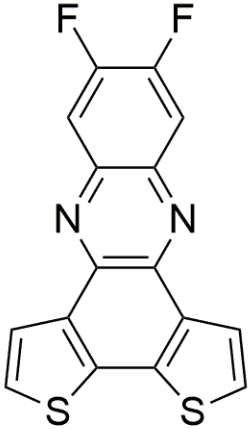
$E^{0/-}$ = -1.79 V[1]

[1] Determined by differential pulse voltammetry in 0.1 M Bu_4PF_6 in dichloromethane

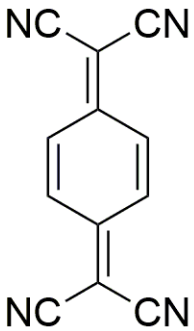
(DTPhz)•TCNQ Donor-Acceptor Co-Crystals Packing



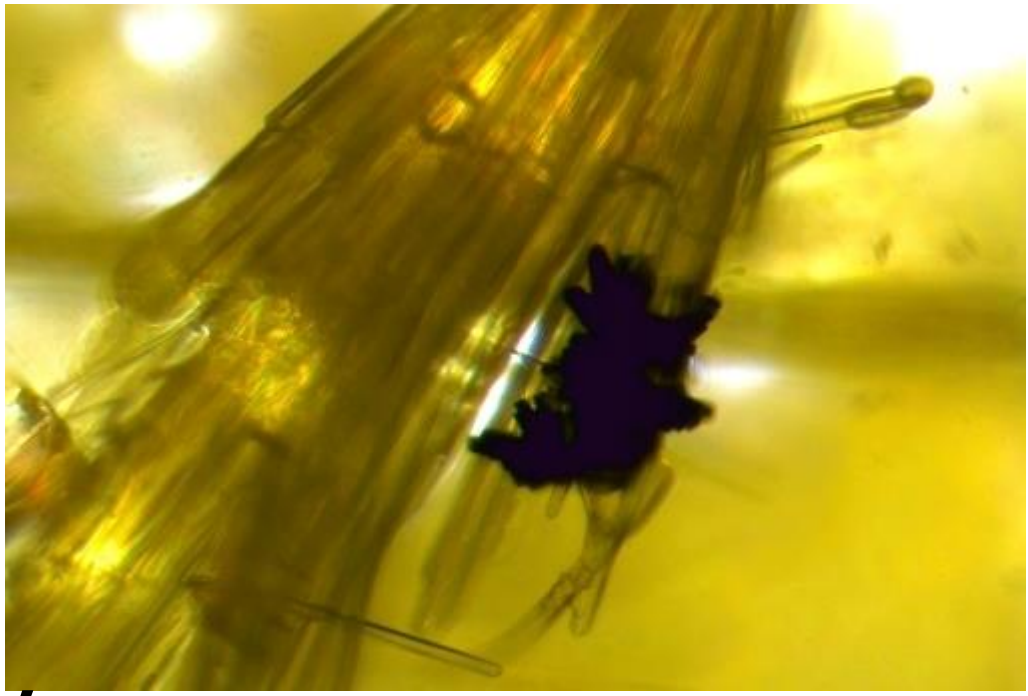
Mixed-Stack Donor-Acceptor (F-DTPhz)•TCNQ Co-Crystals



F-DTPhz



TCNQ

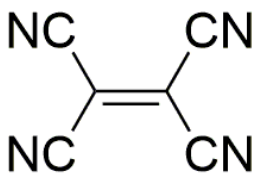


$E^{0/+}$ = +1.16 V[1] $E^{0/-}$ = -0.3 V

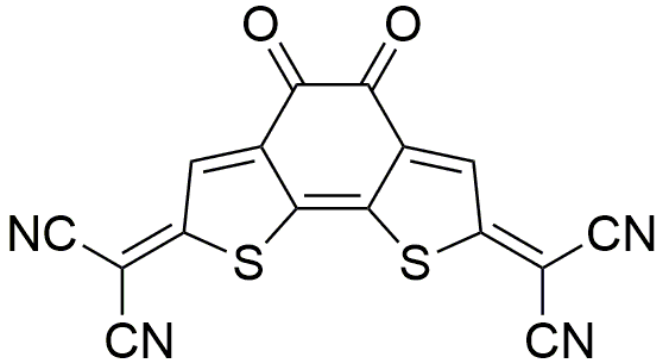
$E^{0/-}$ = -1.72 V[1]

[1] Determined by cyclic voltammetry in 0.1 M Bu_4PF_6 in dichloromethane

Structures of TCNE and Target Acceptor



TCNE



$E^{0/-}$ **= -0.2 V vs** $Cp_2Fe^{+/0}$ **([2])**

[2] Kozaki, M.; Sugimura, K.; Ohnishi, H.; Okada, K. *Org. Lett.*, **2006**, 8, 5235-5238.

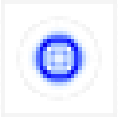
Overview

- What is MEEP? **MIT Electromagnetic Equation Propagation**
- What are the governing equations to be solved? **Maxwell's Equations in 1D, 2D and 3D**
- What is FDTD numerical solution method? **Finite Difference Time Domain**
- What have simulated thus far? **Simple circular geometry (holes) punched through a thin gold substrate. The hole diameter is approximately 100 nm. The excitation signal is from above and directed into the center of the hole. The surrounding boundary condition is air. The plasmon response is plotted as a 2D animated image as well as an output plasmon response data file.**
- What can be varied in the simulation? **Geometry, boundary conditions and material specific dielectric properties**
- Why have we simulated this particular geometry? **It's of interest to see the effects of focusing properties that circular holes and variations on this theme can create by simply varying the geometry or pattern of the holes. Ultimately, the objective is to create nano-tweezers that can manipulate single cells at the nano-scale with great precision. An important tool for biologists doing research in cancer therapy.**

Results

- Geometry

- Animated plasmon response to excitation signal



International Connections

- ITMO, S. Petersburg, Russia
- International Friendship University, Russia
- American University, Beirut, Lebanone

NSF Questions

- What is your plan to address student diversity at all levels: undergraduate, graduate and postdoctoral? ARMAS
- If you do not have a subaward to the partner institution, please explain why not, and how you intend to coordinate travel and student activity with your MRSEC/STC partner. W2
- We are encouraging PREM faculty to obtain release time during the academic year in order to make the PREM research more year round, rather than so strongly focussed on the summer.

INDIRECT DESTRIBUTION – release, equipment, ….

Undergraduate Students

Jose Gallegos 2009 MS Student @ NM Tech

Joseph Torres 2011 MS Student @ U. of Oregon

Jose Herrera 2012 IT specialist @ Bank

Deanna Montoya 2012 Employed @ Bank

Isaiah Otero 2012 MS Student @ NM Tech

Moses Kirui 2012 MS Student @ Florida Tech

Kayla Sawyer 2012 Chemist @ Hospira

Bhupinder Sandhu 2013 PhD Student @ Kansas State U.

Joel Zazueta 2013

Carlos Ordonez 2013 MS Student @ NMHU

Rachael Lucero 2013

Regina Umarova 2015

Graduate Students

Ekaterina Badaeva
2005
Postdoc @ U. of Washington; Engineer at Boeing

Boris Averkiev
2005
PhD @ U. of Utah, Postdoc @ Washington State U.

Ilya Kosilkin
2005
PhD Student @ U. of Washington; Engineer at Boeing

Tiffany Kinnibrugh
2005
PhD @ Texas A&M U.; Argon National Lab

Andrey Yakovenko
2008
PhD @ Texas A&M U.; Argon National Lab

Ernest Asani
2008
Corporate vendor auditor at Leprino Foods Company, Denver, CO

Geetha Bhagavana
2008
INVAGEN pharmaceuticals, Hauppauge, NY

Joseph Mulroy
2009
UNM School of Pharmacy

Kamal Devis
2010
NMHU Business School

Scott Valdez
2010
Employed @ LANL

Nagakeerthi Dasari
2010
Florida

Renuka Tammisetti
2010
Employed @ Pharmacy Store, CA

Graduate Students

Shravana Lakshmi Nayani
2010
Employed at Pharmacy Store, TX

Alexander Romanov
2011
Postdoc University of Eastern Anglia

Alexandr Fonari
2011
PhD Student @ GATech

Praveen Pandi
2011
Neumeric Technologies Corp., OH

Paul Tongwa
2011
PhD Student @ Missouri U. of Science and Technology

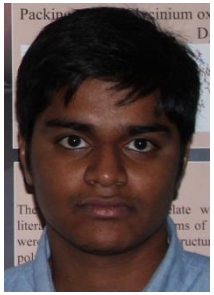
Crystal Ulibarri
2012
Medical Office

Galina Skinner
2012
IT manager, High School, AZ

Samuel Bentum
2013
SABIC Innovative Plastics, Mt. Vernon, IN

Gary Angles
2013
PhD Student @ NM Tech

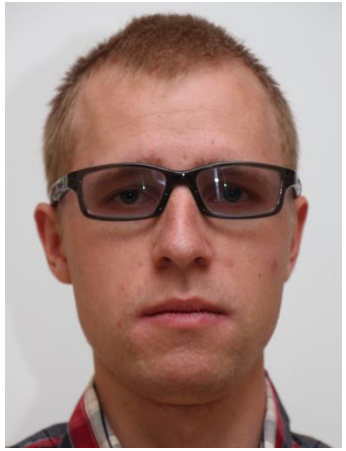
Rene Ebule
2013
PhD Student @ U. of Wyoming



Gnaneswar Elaprolu
2013
Cygtec Inc., Raleigh, NC

Gregory Rael
2014
Taos, high school teacher

Graduate Students



Evgheni Jucov
2014
MS in Computer Science @ NMHU

Carlos Ordonez
2015
IM Flash Technologies, Lehi, UT

Marie Ohoueu
2015
PhD Student @ U. of New Hampshire

Raul Castaneda
2015
PhD Student @ U. of Alberta

Many Thanks for NSF Support and your Attention