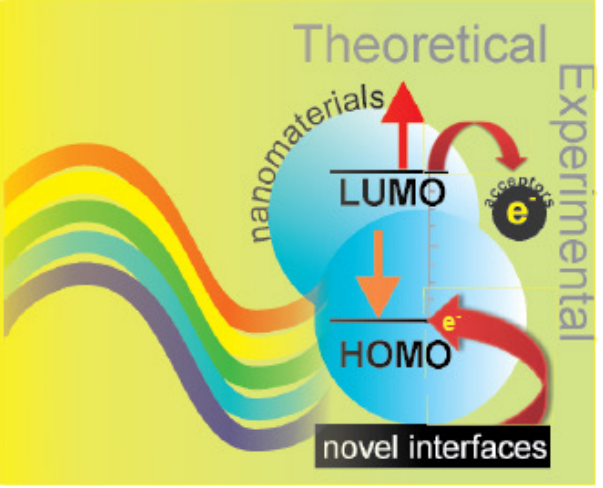
UTEP & UCSB

UNIVERSITY OF CALIFORNIA
SANTA BARBARA

PREM

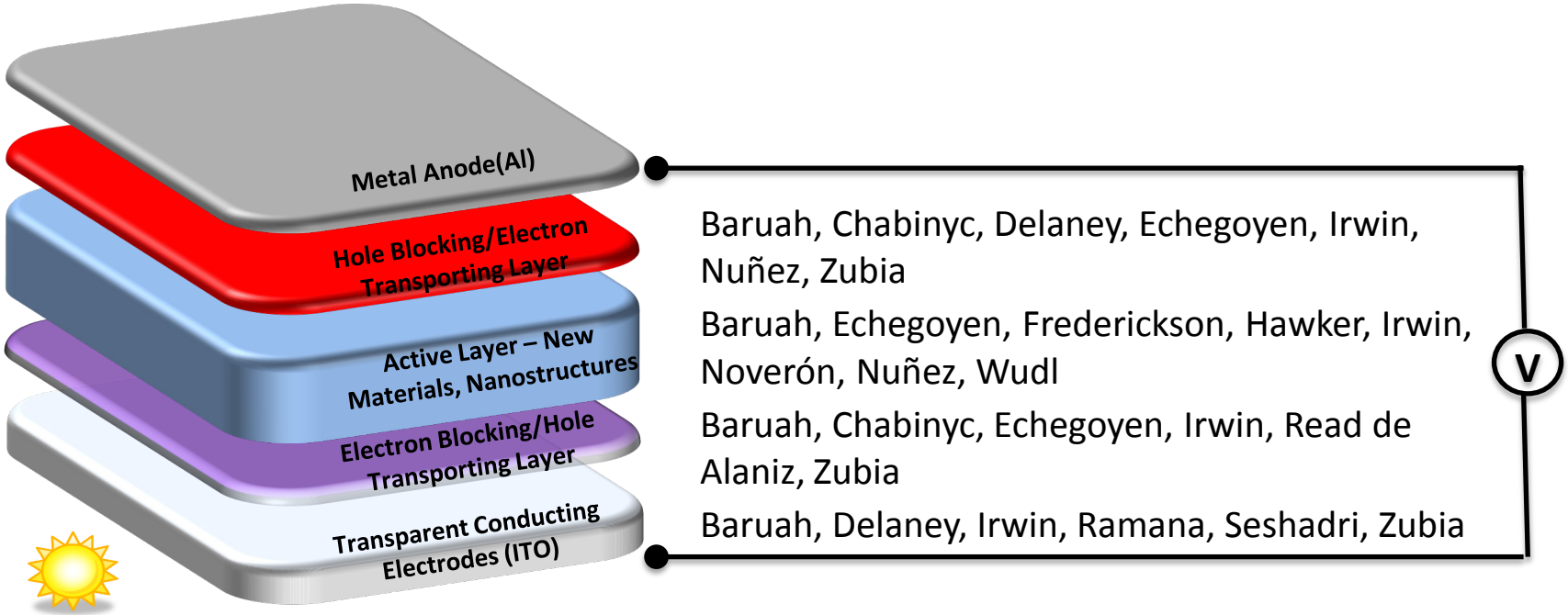


Fundamental Molecular and Interfacial Design for Next Generation Photovoltaic Systems

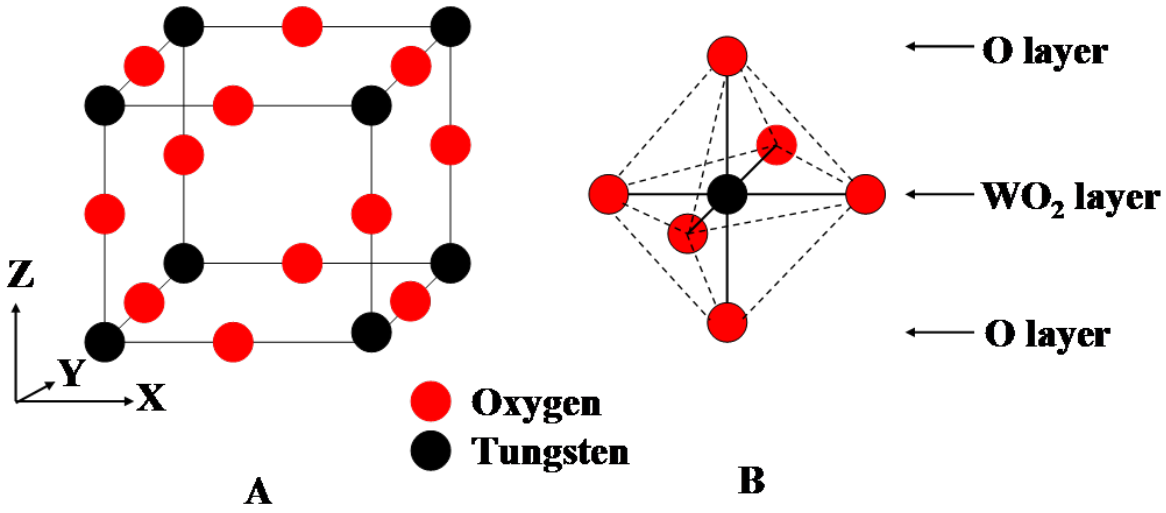
PREM People and Concepts

Luis Echegoyen – PI - Chemistry
Tunna Baruah - Physics
Gabby Gándara - Engineering
Michael Irwin - Chemistry
Juan Noverón - Chemistry
José Nuñez - Chemistry
Chintalapalle Ramana (Mech. Eng.)
David Zubia – Elec. Eng.

Craig Hawker – co-PI - Materials
Michael Chabinyc - Materials
Kris Delaney - Materials
Glenn Fredrickson – Chem. Eng.
Dorothy Pak - Materials
Javier Read de Alaniz - Chemistry
Ram Seshadri - Chemistry
Fred Wudl - Chemistry

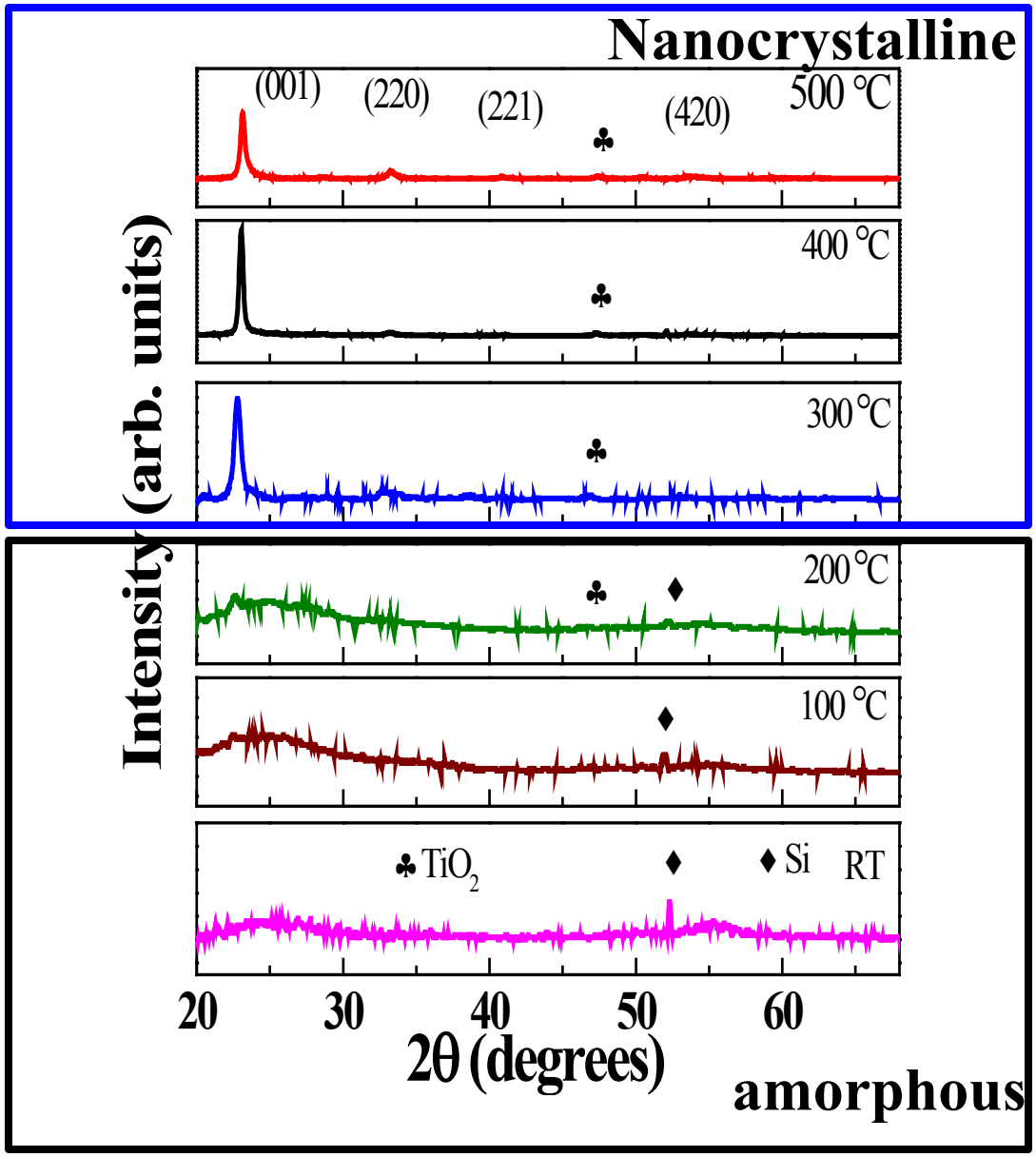


Investigation of Indium Free Transparent Conducting Oxides for Application in Photovoltaics (C. V. Ramana and R. Seshadri - leaders)



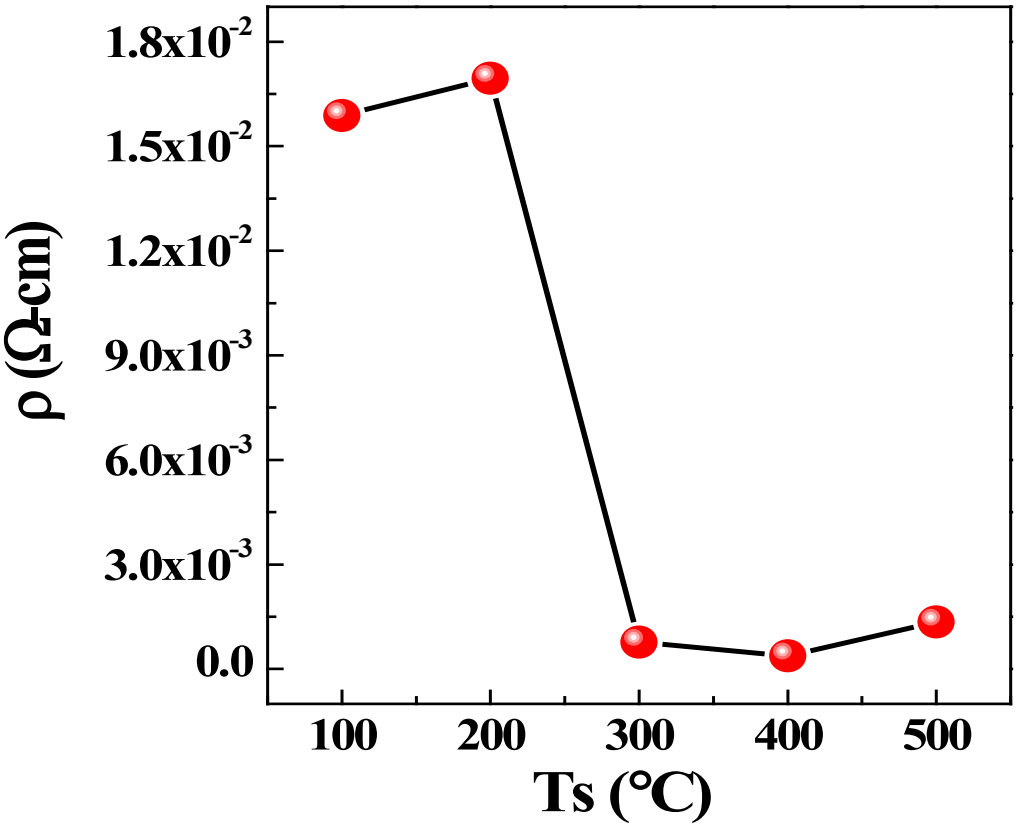
Phase	Symmetry	Temperature Range (K)
$\alpha - WO_3$	Tetragonal	1010 – 1170
$\beta - WO_3$	Orthorhombic	600 – 1170
$\gamma - WO_3$	Monoclinic	290 – 600
$\delta - WO_3$	Triclinic	230 – 290
$\varepsilon - WO_3$	Monoclinic	0 - 230
Source: P. A. Cox, *Transition Metal Oxides, 1995* (Oxford)		

W-Ti-O Thin Films – Structure



N.R. Kalidindi et el., *ACS Appl. Mater. Inter.* (2011)

W-Ti-O Thin Films – Electrical



N.R. Kalidindi et el., *Appl. Phys. Lett.* (2010)

Theoretical Work Already Started - Delaney

Summary

WO_3 surface (in progress):

- Work function vs. interface orientation
- Reconstructions & surface termination
- Surface gap states

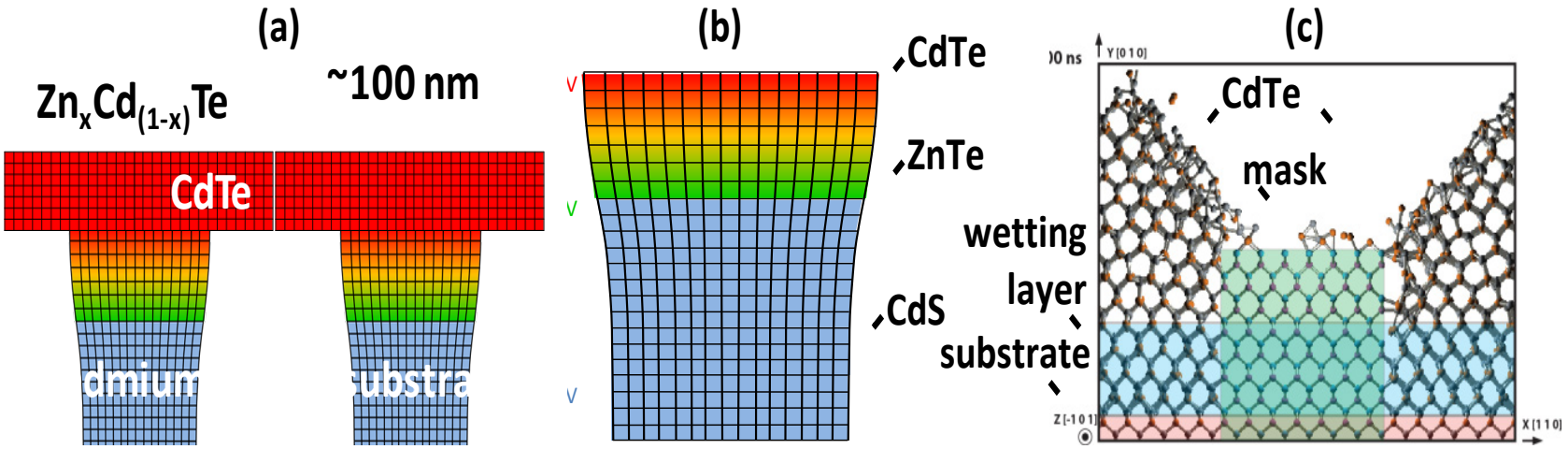
WO_3 conductivity:

- Electrical character & E_{form} of Ti doping
- Alternative dopants, especially *p*-type

WO_3/P3HT interface:

- Donor/anode interface alignment vs. orientation
- Structure optimization?

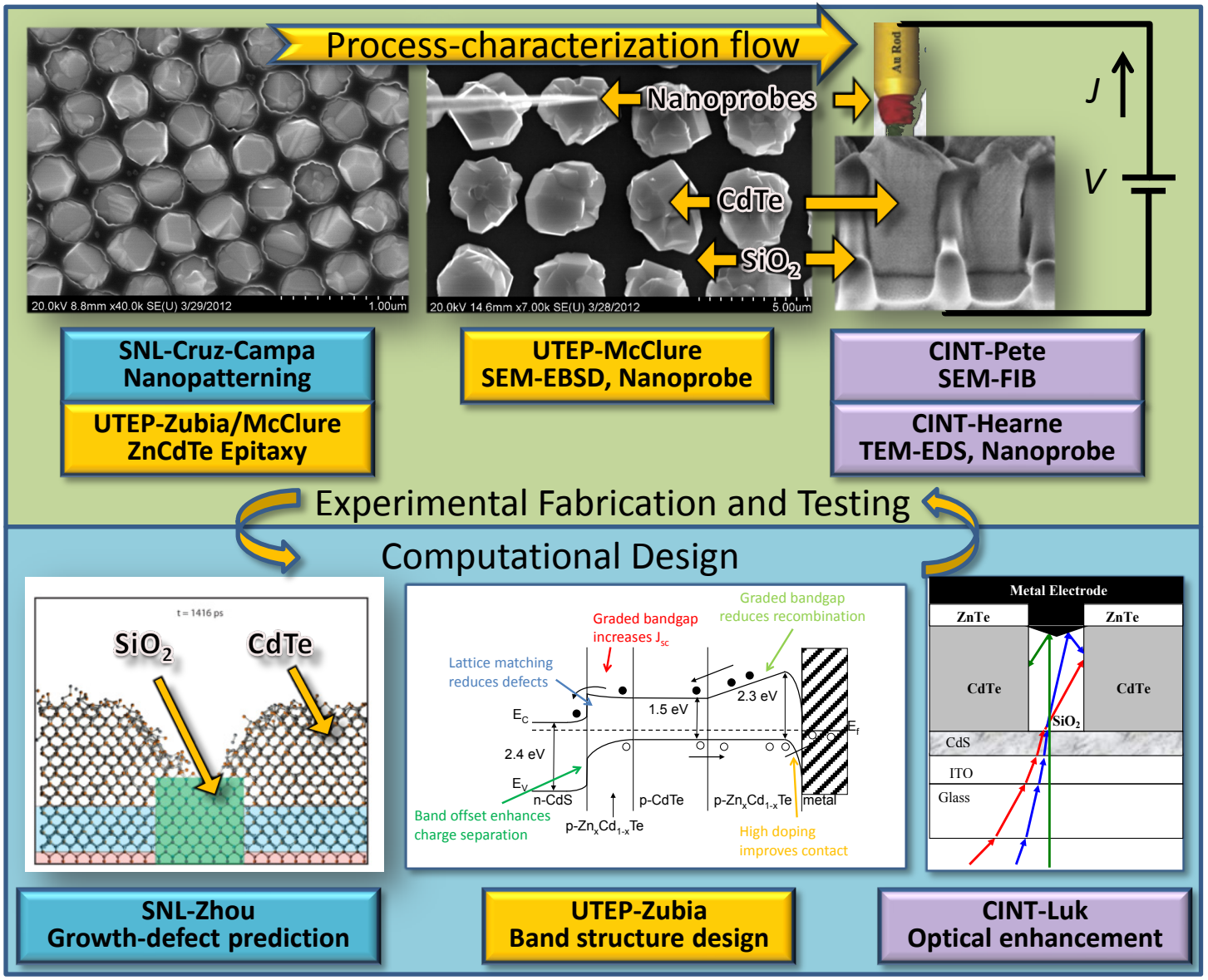
Molecular Dynamics Simulation of Strained, Nanoscale Crystal Growth using Bond Order Potentials (D. Zubia, X. Zhou, and K. Delaney - leaders)



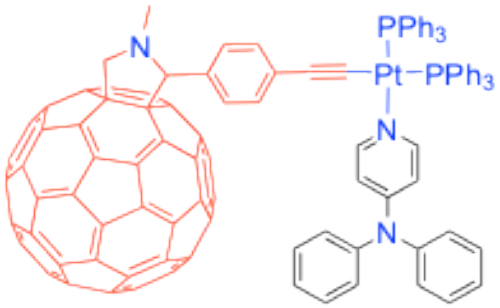
(a) Strained, nanoscale crystal growth of ZnCdTe on CdS, (b) 3D strain partitioning in ZnCdTe/CdS, (c) MD bond-order potential simulation of 10% strained, selective-area growth of CdTe.

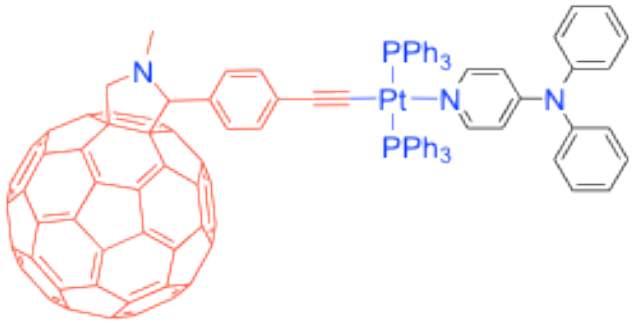
Concept and Methodology

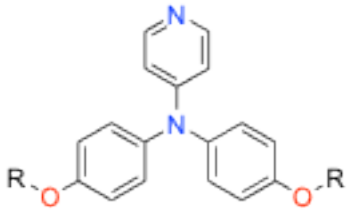
Comprehensive Experimental and Simulation Aspects

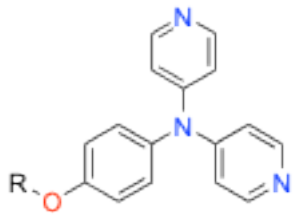


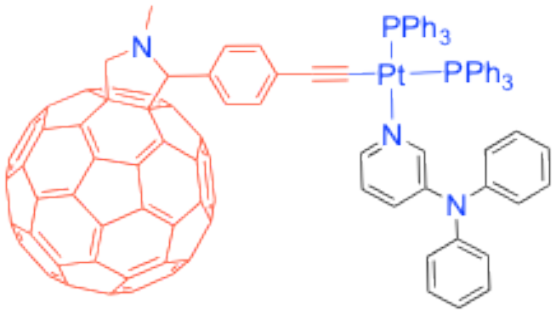
σ-Alkynyl Complexes of Platinum and Pyridine Amines as Potential Photovoltaic Materials. (J. Nuñez and J. Read de Alaniz - leaders)

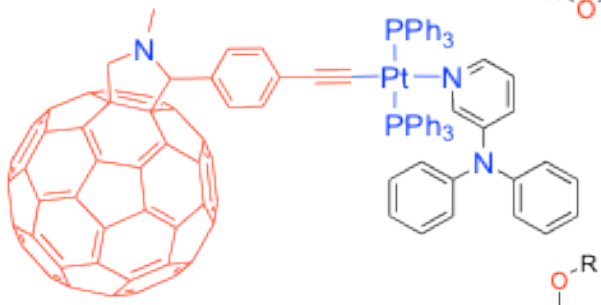


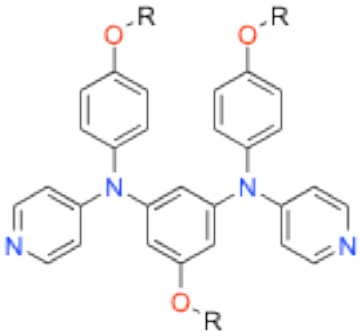


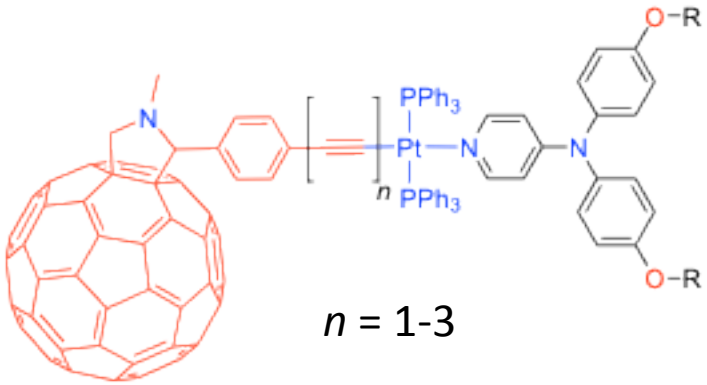




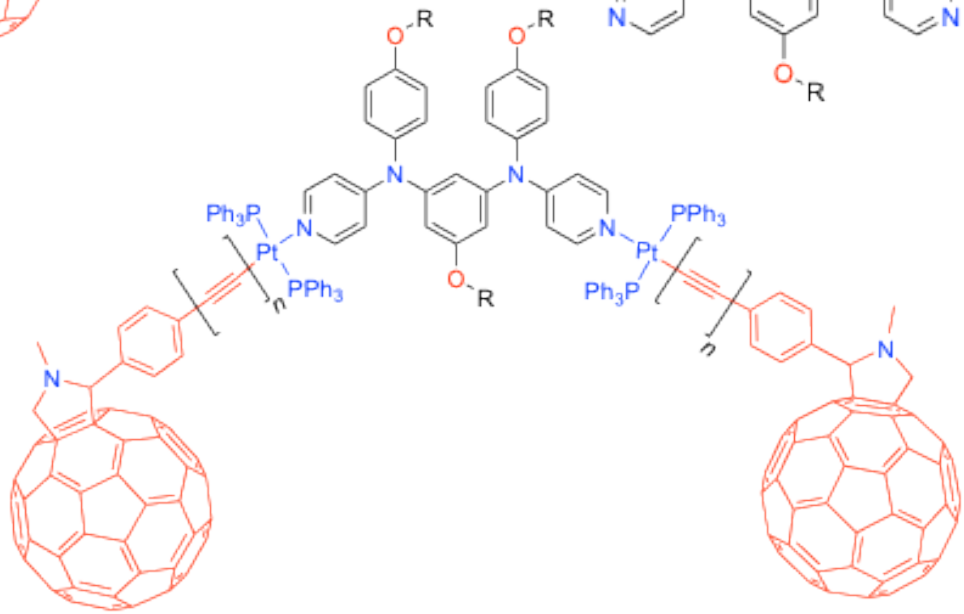




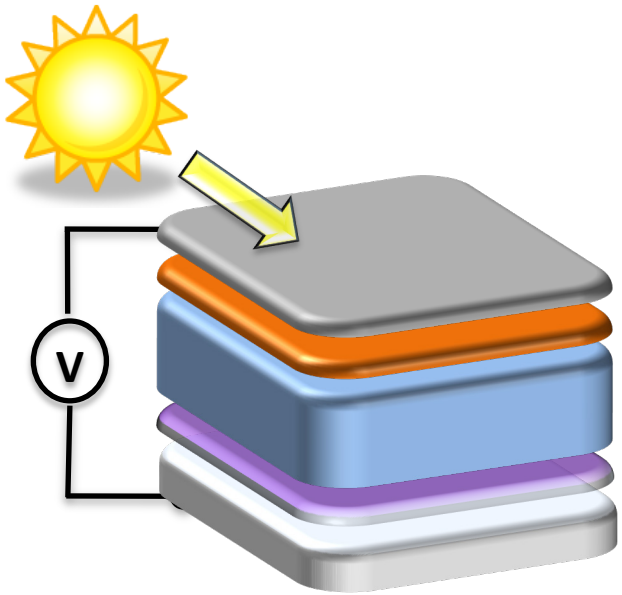


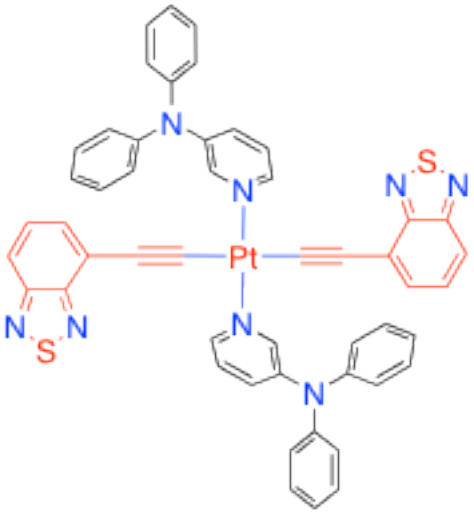


n = 1-3

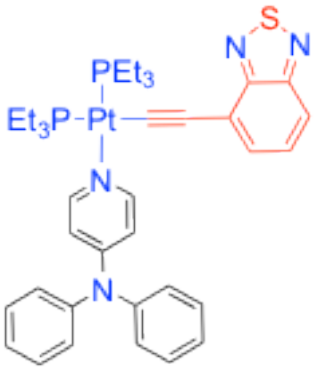


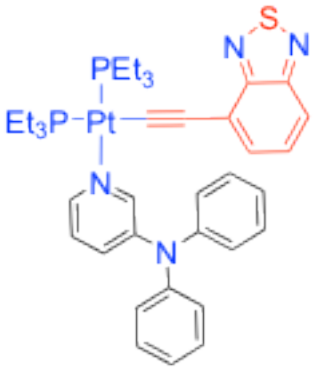
Future work

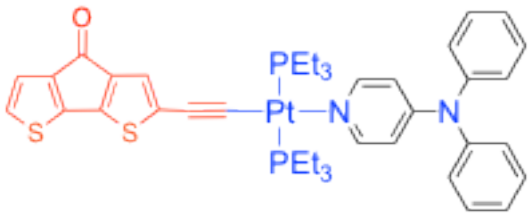


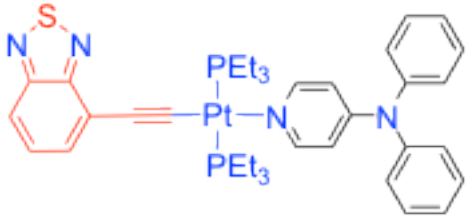


Other targets



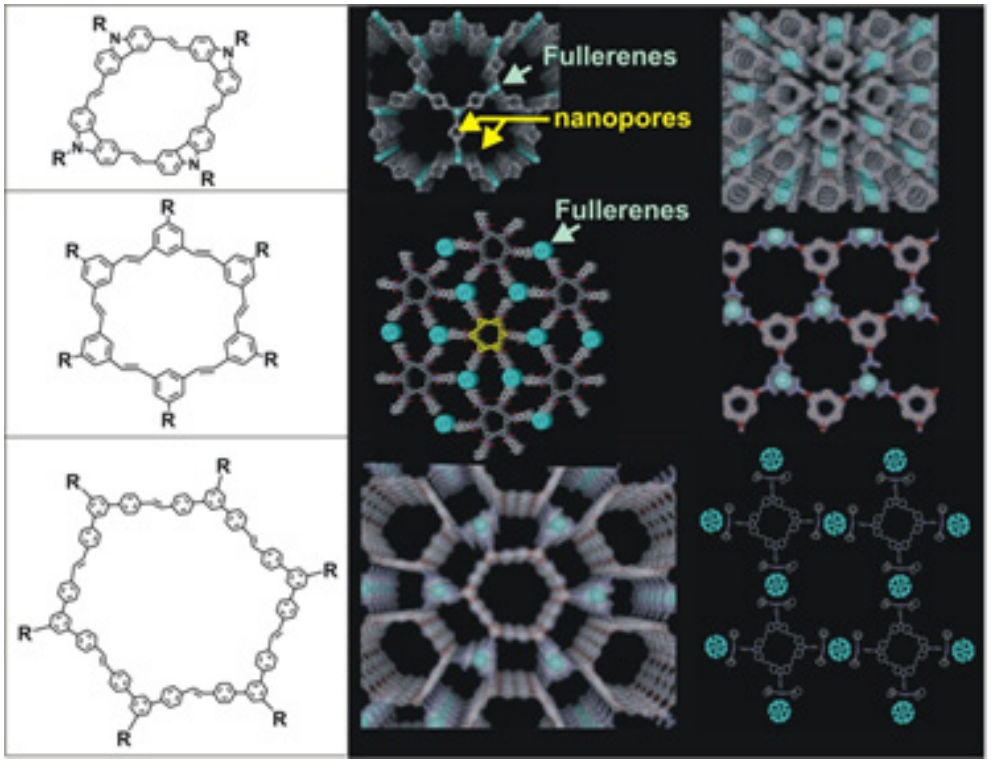


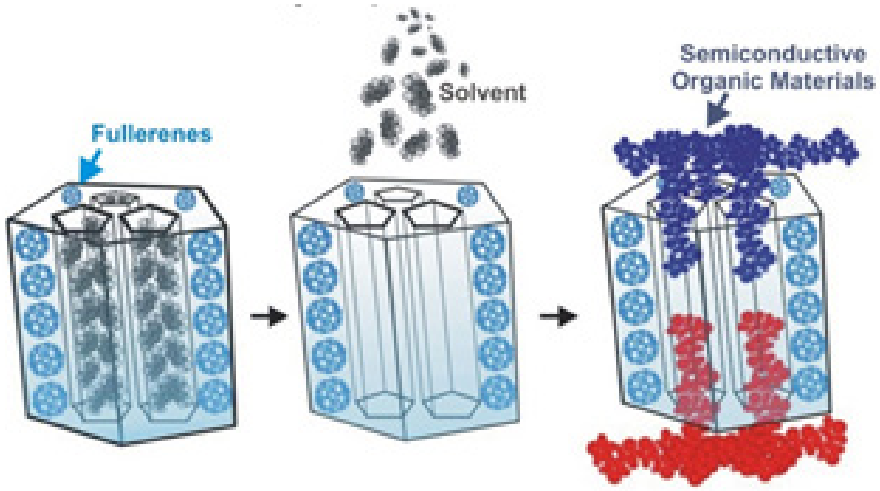




Novel Fullerene Nanostructures and Heterojuction Interfaces (J. Noverón and C.J. Hawker - leaders)

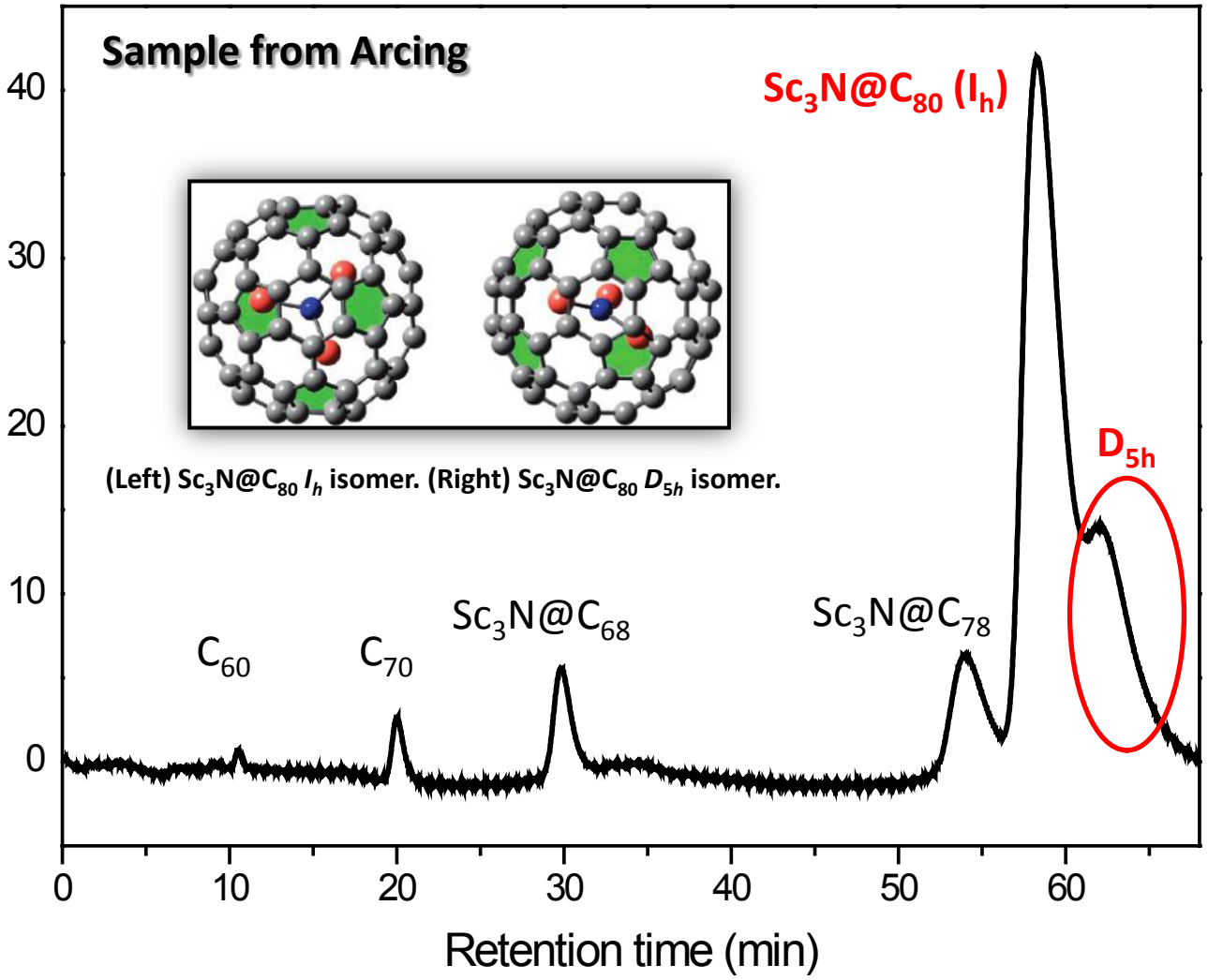
Crystalline fullerene systems designed with large porosities expected to be solvent-filled, and upon desolvation, may allow for post-assembly inclusion structures with semiconductor materials

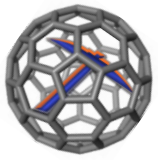




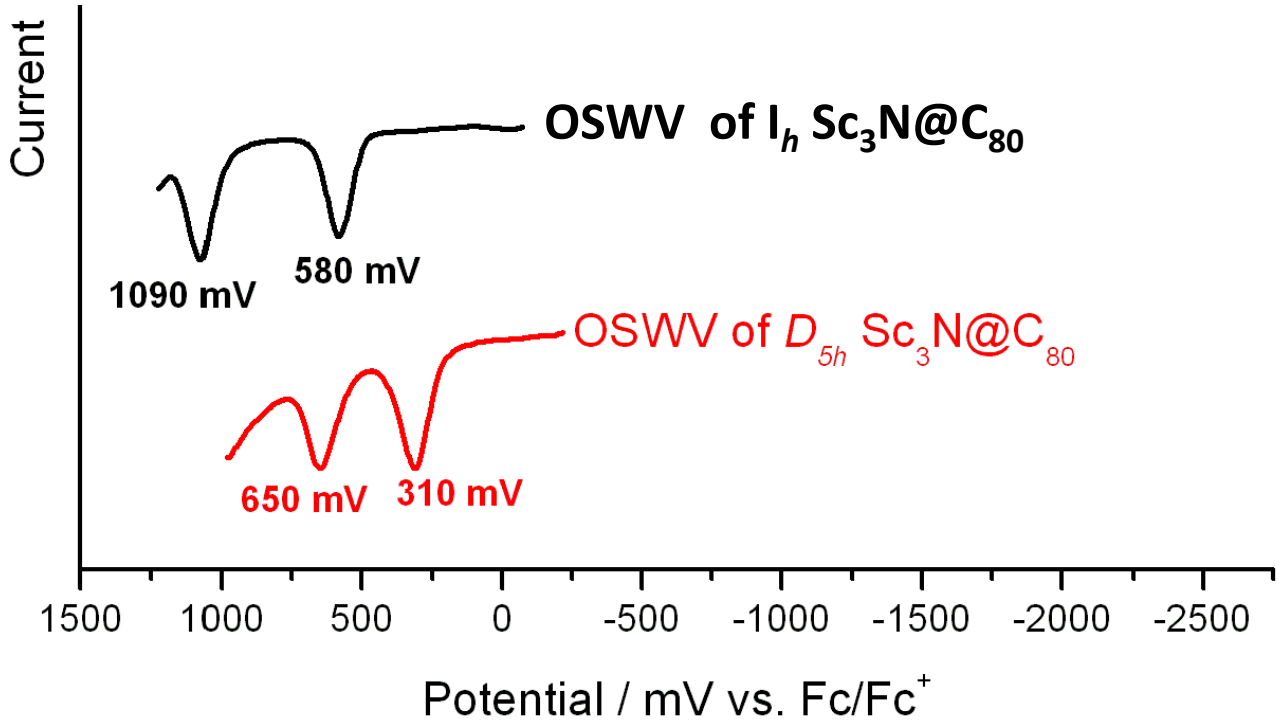
Redox-Based Methods to Prepare Macroscopic Quantities of New Endohedral Fullerenes and their Derivatives for Photovoltaics (PV) (L. Echegoyen and F. Wudl - leaders)

Isomeric Separation of I_h and D_{5h} $Sc_3N@C_{80}$ by Selective Chemical Oxidation



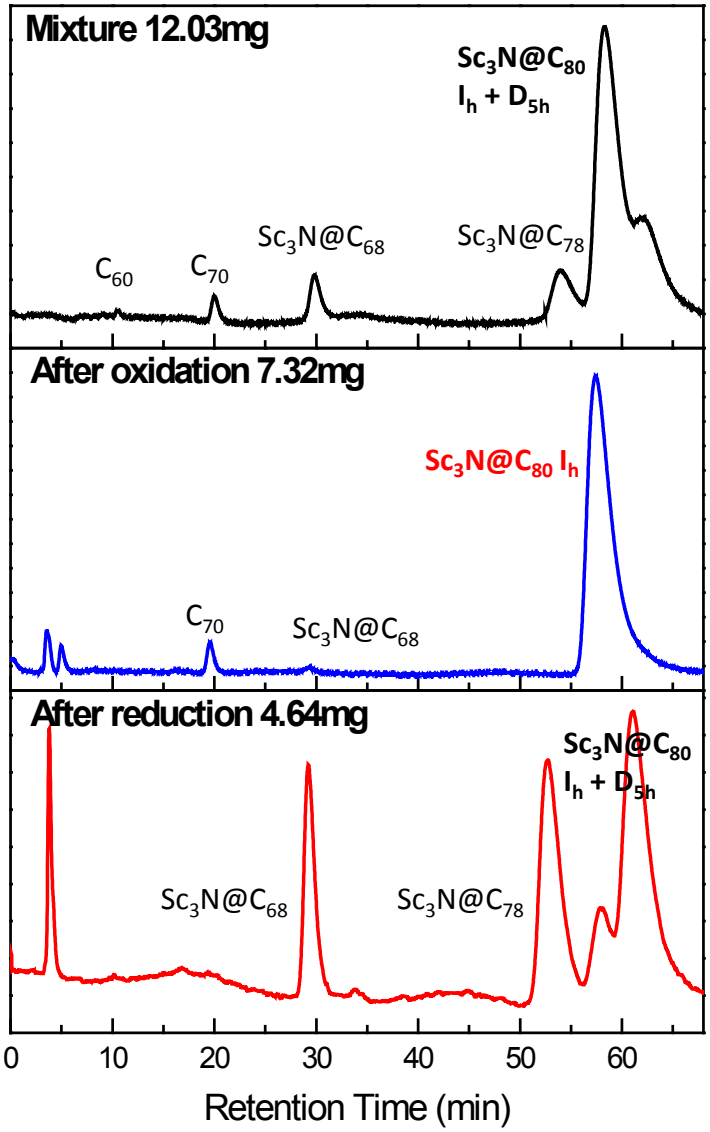


OSWV of I_h and D_{5h} $Sc_3N@C_{80}$



Stevenson, Mackey, Coumbe, Phillips, Elliott, and Echegoyen
J. Am. Chem. Soc., 129, 6072-6073, **2007**

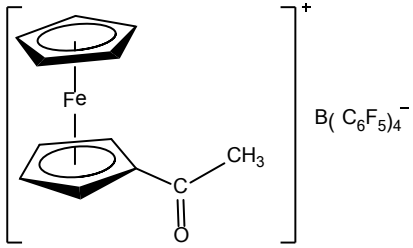
Isomeric Separation of I_h and D_{5h} $Sc_3N@C_{80}$, and $Sc_3N@C_{78}$ by Selective Chemical Oxidation



Mixture @C_{80} 65.44% I_h + 24.20% D_{5h}

@C_{78} 6.09%, @C_{68} 3.45%
C_{70} 0.62%, C_{60} 0.20%

with 11.02mg salt



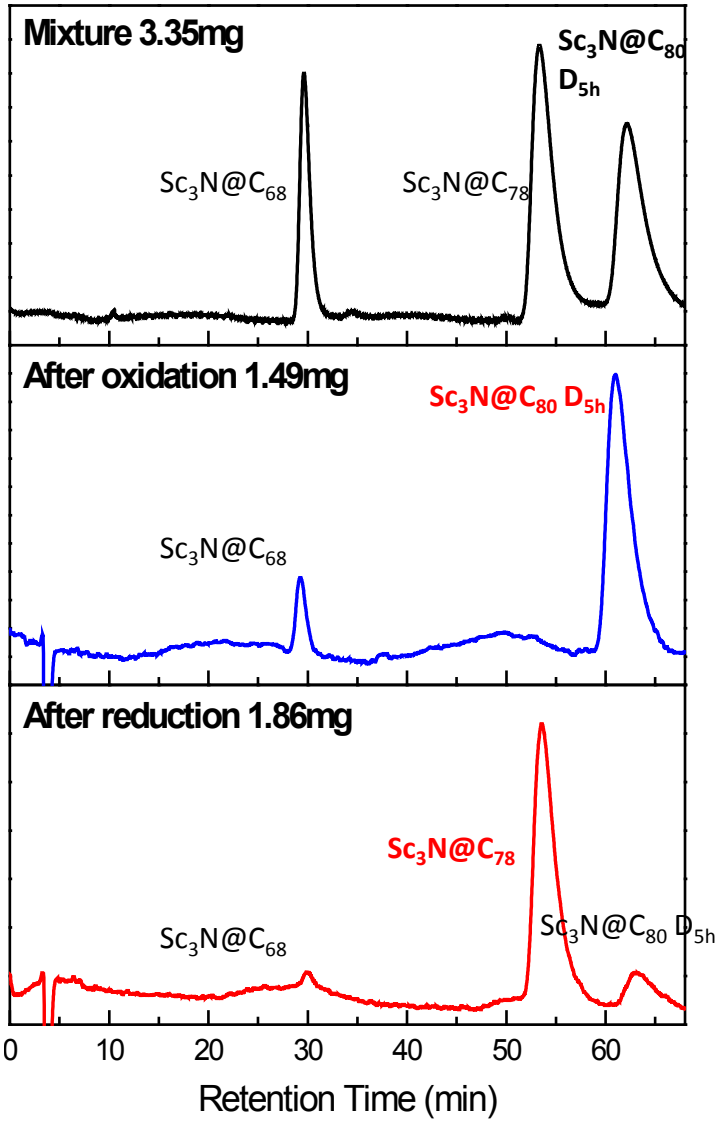
Oxidation 1 @C_{80} 94.52% I_h

@C_{68} 0.38%, C_{70} 5.10%

Reduction 1 @C_{80} 8.58% I_h + 39.27% D_{5h}

@C_{78} 26.67%, @C_{68} 26.03%

Isomeric Separation of I_h and D_{5h} $Sc_3N@C_{80}$, and $Sc_3N@C_{78}$ by Selective Chemical Oxidation



Mixture @C_{80} 37.92% D_{5h}

@C_{68} 7.39%, C_{78} 54.69%

with 2.58mg salt

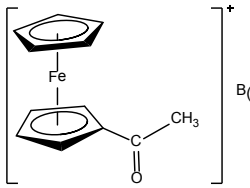
Oxidation 3 90.52% D_{5h}

@C_{68} 9.48%

Reduction 3 @C_{80} 7.50% D_{5h}

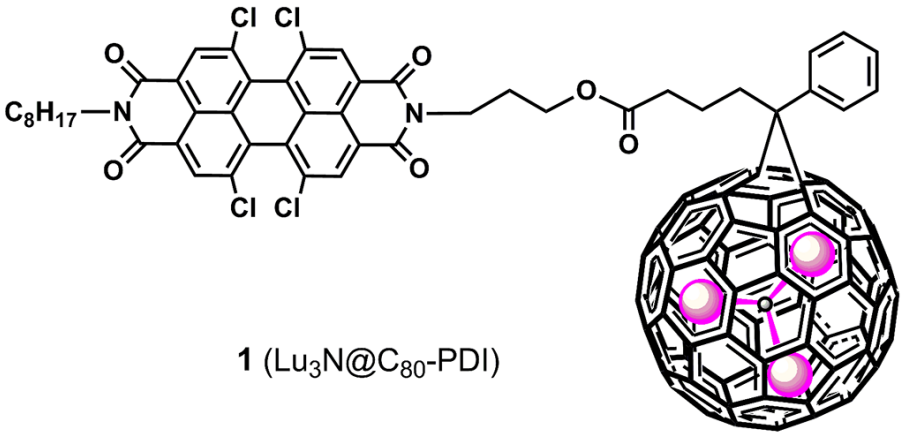
@C_{68} 1.34%, C_{78} 91.16%

Fullerene	E_p^{ox} (V) vs Fc/Fc^+
$Sc_3N@I_h$-C_{80}	0.59
$Sc_3N@D_{5h}$-C_{80}	0.32
$Sc_3N@D_3$-C_{68}	0.33
$Sc_3N@D_{3h}$-C_{78}	0.21

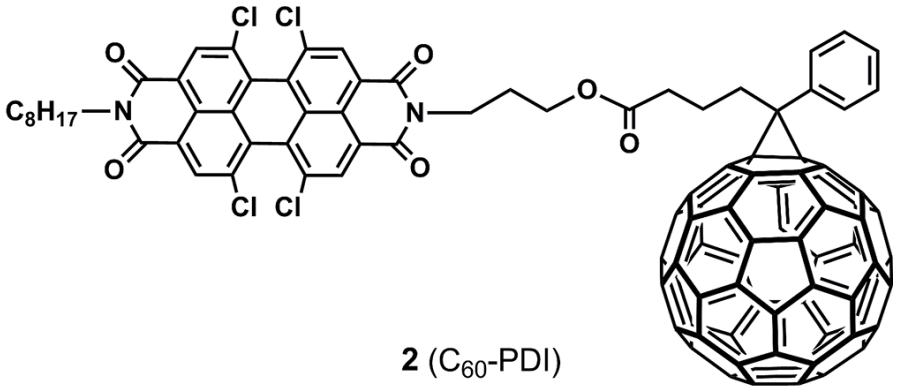


0.27 V

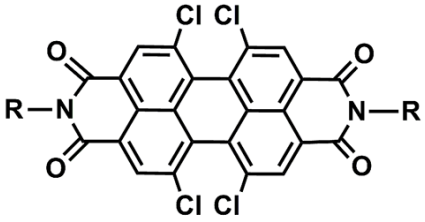
Fullerenes as Donors in Organic Solar Cells?



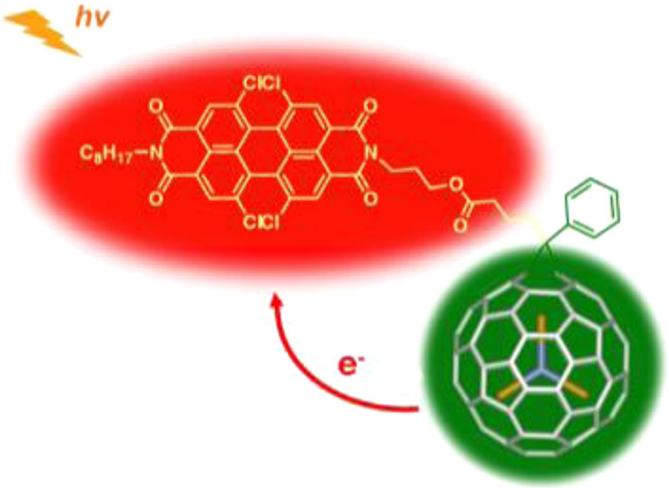
1 ($Lu_3N@C_{80}$-PDI)



2 (C_{60}-PDI)



8: R = $-C_8H_{17}$
11: R = $-C_5H_4N$



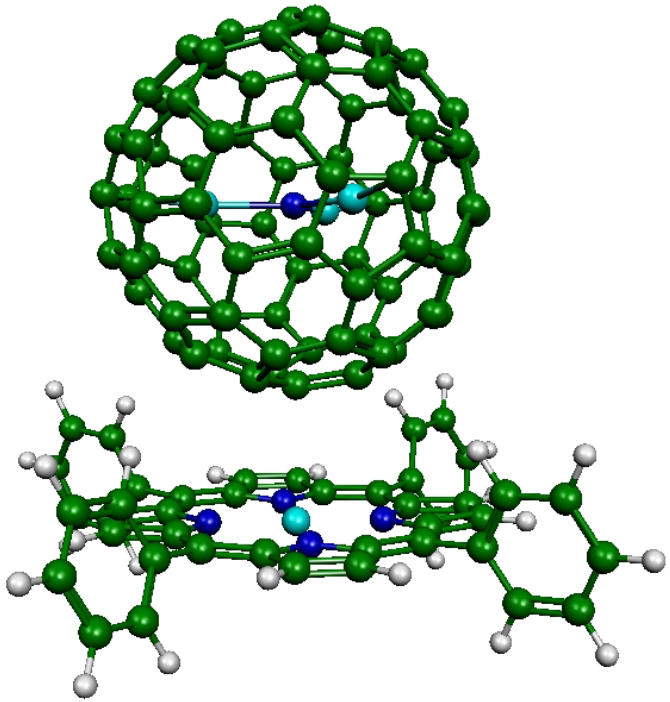
Feng, Rudolf, Wolfrum, Troeger, Slanina, Akasaka, Nagase, Martín, Ameri, Brabec, and Guldi
J. Am. Chem. Soc. **2012**, *134*, 12190−12197

Simulation of Charge and Energy Transfer in Organic Photovoltaics (T. Baruah and K. Delaney - leaders)

Work in progress/proposed :

- Model donor-acceptor systems with endohedral $Sc_3N@C_{80}$ fullerene as acceptor : Electronic structure.
- Fullerene derivatives as acceptors: changes in electronic structure and CT energies.
- Solvent polarization for DA molecular conjugates – effect on the CT states.
- Energy transfer rates in DA complexes.
- Small clusters of doped WO_3 – its electronic structure and optical properties.

Sc_3NC_{80}-TPP and $Sc_3N@C_{80}$-ZnTPP Model Compound



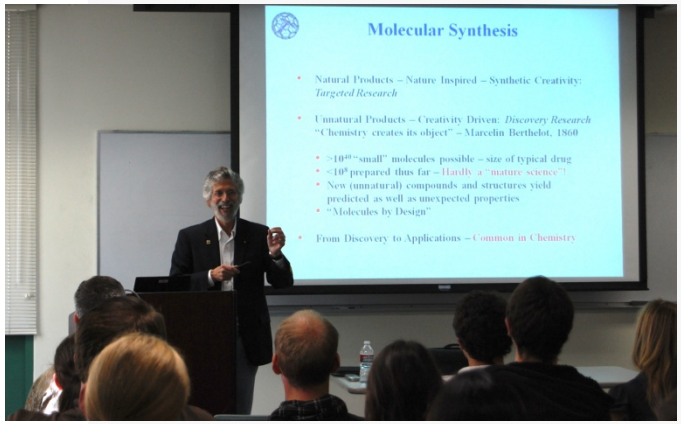
- Two conformers of each complex are being studied.
- Figure shows an optimized conformer with ZnTPP facing a 6:6 bond of the fullerene. The complex was optimized at the all-electron generalized gradient level.
- Center-to-center separation: 7.35 Ang.
- DFT HOMO-LUMO gap: 1.05 eV (underestimated in DFT, not actual gap)
- Ground state dipole moment : 0.6 Debye (from fullerene to ZnTPP).
- Further calculations on IP, EA, CT energetics are in progress.

Education and Outreach

(Gabby Gándara and Dorothy Pak)

University of California - Santa Barbara
University of Texas at El Paso

Research Experiences for Undergraduates



- Exchange UCSB and UTEP undergraduates for summer REU programs (4 in each direction)
- Mentored research experiences in PREM research groups (Summer 2012: 15 interns in UCSB PREM labs)
- UTEP students included in RISE/CAMP internship cohort
- Participation in skills development and career development workshops and seminars

UCSB-UTEP Undergraduate Colloquium

Connect UTEP and UCSB undergraduates to increase awareness of opportunities at partner institution

- Annual end-of-summer poster session
- Alternate between UCSB and UTEP site
- At UTEP – in connection with COURI Symposium

Materials Science Ambassadors

- PREM graduate students assist with K-12 outreach activities at local schools – based on UTEP program, to be launched at UCSB
- It's a Material World - UCSB
- Build-a-Buckyball and Solar Car Workshops - UCSB

Outreach Programs

Materials Science Ambassadors	• Develop Relationship with Math/Science Teachers • Service Learning • Nexus - Research Shadowing Program
ExciTES Summer Institute	• Summer Camp for 6th – 10th graders • Modular Inquiry-based, Team-based Activities
Materials Research Outreach Program	• Grad and postdoc poster session • Meeting and engaging industrial partners

ExciTES = Excellence in Technology, Engineering and Science

Evaluating the Impact of our Programs

Metrics of success

- REU evaluation using URSSA instrument
- Participants continue on to graduate school in science and engineering
- Participants enroll in graduate school at partner site
- Undergraduates participate in conferences and publications
- Graduate students participate in K-12 outreach