

**Professor Alejandro D. Rey, Eng., PhD, FRSC (UK), FASP**  
**RESEARCH PROGRAM SUMMARY ■ COMPUTATIONAL MATERIALS SCIENCE**  
**Theory ■ Modeling ■ High Performance Computing**

Bio-mimetic-based Green Mfg.	Interfacial processes in bio & food colloidal systems.	R Mezzenga , ETH-Zurich Switzerland	FQNRT NSERC NSF
	Design and Characterization of Multi-component Protein-Based Fibers	Justyn Jaworski, Dept. of Bioengineering, U Texas Arlington	
	Plant cell walls – simulation of self –assembly and growth as a <b>model for green composites’ manufacturing.</b>	D Pasini, (Physics) & T Western (Bio). McGill	
	Biospinning/molding - Spider Silk - Study of structural/functional relationships of <b>biomimetic proteins genetically engineered, production of material from the proteins</b> , mathematical modeling complex fluid flow dynamics in natural & a spider duct-mimetic system = <b>design of biomimetic production processes.</b>	J von Oehsen, CoES & M. S. Ellison, MSE (Polymers), Clemson U, SC; EE H Valencia, UNAM, México	
Energy Storage materials	<b>Gas hydrates modeling of methane/hydrogen storage</b> in clathrates for <b>safe &amp; efficient energy storage</b> based on molecular level understanding.	Phil Servio (Chem. Eng.) McGill	PRF NSERC
	Hydrogen Storage - <b>metal-loaded activated carbon microfibers</b> ; electronic calculations/molecular dynamics elucidate interactions between carbonaceous pitches & metal particles - believed to provide <b>hydrogen storage enhancement.</b>	Dan Edie, CAEFF, Clemson SC & N. C. Gallego, Carbon Mat. Tech. Group, Oak Ridge, TN	NSF CAEFF
Structural and Functional Materials	Nanocomposite Liquid Crystals – Modeling free surfaces & confinement - presentation of a <b>comprehensive rheological characterization of liquid crystalline materials</b> using computer simulation.	E Soulé & M Aranguren, INTEMA, Argentina; Reven, Lennox & Sutton OCAM - McGill	PRF NSF CAEFF US AIR FORCE DOE DUPONT NSERC FCAR FQNRT
	<b>Liquid crystal electro-optics-modeling</b> novel molecular architectures for next generation display and <b>solar energy devices.</b>	M Srinivasarao, Georgia Inst. Tech GA & Satyendra Kumar, Kent State, OH	
	Kevlar Fibers - multi-scale multi-transport modeling of fibre formation with <b>predictable structure/property relations.</b>	Dr. Allred, DUPONT	
	Systems-oriented study of <b>carbon &amp; polymer fibres &amp; films</b> → computational models integrating molecular information with continuum or microscopic-level models & produced <b>advanced visualization tools FISYM</b> - a ‘kit’ for polymers & flow-induced crystallization.	Dan Edie & A.S. Ogale, (CAEFF/NSF/MIT) Kostya Kornev (COES) Clemson U, SC	
Bio-Materials	Biosensors - A <b>new elasto-optics methodology</b> was developed & applied to describe the performance of a <b>new generation of protein &amp; virus biosensors</b> based on “liquid crystal vision.”	Nick Abbott U Wisconsin - Madison	NSERC
	<b>Flexoelectric membranes</b> - modeling mechano-transduction in biological membranes with applications to <b>the physiology of hearing and to flexo-based sensors and actuators.</b>	Dr. W. E. Brownell, Cochlear Biophysics Lab, Otolaryngology, Baylor School of Medicine, Houston TX	
	Biofilms- coupled <b>bio-mechanical modeling of cell population growth.</b>	CAMBAM /McGill	
Commodity Polymers	Polyethylene - Phase separation in compressible polymer solutions <b>introduced new static &amp; kinetic couplings never previously studied.</b>	Dr. Eric Cheluget NOVA, AB	NOVA NSERC