Colección Memorias de los Congresos de la Sociedad Química de México
52° Congreso Mexicano de Química Y 36° Congreso Nacional de Educación Química
Sociedad Química de México A.C.
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Conferencias Magistrales

"Transforming the Periodic Table: Catalysis with Earth Abundant Transition Metals"

Prof. Paul J. Chirik
Department of Chemistry, Princeton University

Modera: Dra. Itzel Guerrero Ríos. Facultad de Química, UNAM.
Miércoles 27 de Septiembre Horario: 10:30-11:30 Salón: Rivera + Siqueiros

Biosketch

Doctor of Philosophy, Chemistry April, 2000, California Institute of Technology, Pasadena, CA.
Advisor: Professor John E. Bercaw.
Dissertation: Ancillary Ligand Effects on Fundamental Transformations in Metallocene Catalyzed Olefin Polymerization.

Most Synergistic Activities

Editor-in-Chief, Organometallics, Associate Director for External Partnerships, Andlinger Center Chair, Inorganic Reaction Mechanisms Gordon Conference.

Abstrac

Transition metal catalysis has revolutionized modern society by enabling new chemical transformations with unprecedented activity and control over selectivity. Applications range from new silicone materials to transforming hydrocarbons into fuels to building blocks for pharmaceuticals. Our laboratory has been actively engaged in developing catalysts based on earth abundant, first row transition elements rather than more traditionally deployed precious metals that are some of the least available elements in the Earth's crust. Use of these elements extends beyond potential cost advantages; reduced carbon dioxide production and stability of supply chains are also potential benefits. Ultimately we aim to discover new reactivity that exploits the unique electronic structures of first row transition metals. My lecture will combine applications developed in combination with industrial collaborators and focus on the multifaceted challenges of transitioning from the academic laboratory to processes used on scale. Earth abundant catalysts for commercial silicone production,1 asymmetric alkene hydrogenation,2 C-H functionalization3 and radiolabeling of pharmaceuticals4 have been developed. More recently we have been focused on the discovery of new catalytic reactions for the upgrding of simple alkenes – those that are now readily available due to the development of shale gas reserves. An iron-catalyzed method for the diastereo- and regioselective intermolecular [2+2] cycloaddition of commodity alkenes has been discovered and opens new molecular space within fundamental hydrocarbons (Figure 1).5 Through continued ligand evolution and understanding of electronic structure, we have discovered base metal catalysts that promote chemistry unknown with established precious metal variants. The mechanisms of the various catalytic transformations, the importance of electronic structure controlled through ligand manipulation and strategies for imparting air stability will be a highlighted throughout.

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Figure 1: Unique [2+2] cycloadditions of ethylene and butadiene promoted by iron catalysts.

Acknowledgements: We thank the US National Institutes of Health (R01 GM121441) for financial support.

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2.Friedfeld, M. R.; Shevlin, M.; Hoyt, J. M.; Krska, S. W.; Tudge, M. T.; Chirik, P. J. Science, 2013, 342, 1076.
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Agradecemos a la American Chemical Society por el apoyo otorgado para la participación del plenarista.

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"Some new developments in density functional theory for calculating and analyzing inter and intramolecular interactions"

Prof. Martin Head-Gordon
Kenneth S. Pitzer Center for Theoretical Chemistry,
Department of Chemistry, University of California, and Chemical Sciences Division, Lawrence Berkeley National Laboratory

Modera: Dr. Alberto Vela Amieva. Centro de Investigación y de Estudios Avanzados.

Jueves 28 de septiembre Horario: 9:30-10:30 Salón: Rivera + Siqueiros

Biosketch

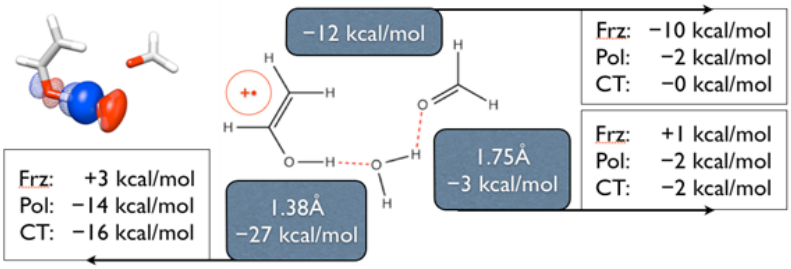
Professor Head-Gordon's group performs research on the development and application of electronic structure theories, to permit the treatment of problems that are currently beyond the reach of standard methods. The electronic structure problem is to calculate the properties of a molecule from first principles quantum mechanics, with the objective of obtaining information on structure and reactivity. Rereach group.

Our research centers on the development and application of methods that predict the electronic structure of interesting molecules. Exciting progress has occurred over the last decade to the extent that many ground state molecular properties are accurately and routinely calculated. In cases of exotic transient species, theoretical approaches can in fact be the most feasible tool available. We seek to open new classes of chemical problems to study via electronic structure theory. Realization of this goal generally requires the coupling of fundamental quantum mechanics with large scale scientific computing.

Electronic structure theory is broad in scope with existing connections to many branches of experimental chemistry, and the potential for many more. Interesting molecules may range from diatomics through medium sized organic and inorganic species to adsorbate-surface systems. The molecules may be in their ground electronic state or they may be electronically excited. Time-independent properties such as geometric structure and relative energies are often of interest, or we may be concerned with transitions between levels and dynamical processes.

Abstrac

Density functional theory (DFT) is the most widely used electronic structure theory. Crucial to its future is the problem of designing functionals with improved predictive power. I shall describe a new approach to functional design, "survival of the most transferable", and show how the resulting functionals offer unprecedented accuracy for DFT calculations of intermolecular interactions. As a counterpoint to this vital numerical development, I will discuss the challenge of obtaining physical insight into DFT calculations of intermolecular and interactions. We are aiming to meet this challenge with new energy decomposition analysis (EDA) methods that separate interactions associated with frozen fragment electronic structure, from induced electrostatics, and forward and backwards charge transfer. I will present a variety of examples, such as the triplex between vinyl alcohol radical cation, formaldehyde and water, which is a rearranged form of the glycerol radical cation. Finally I will consider chemical bonds, where spin-coupling between electrons must also be explicitly accounted for.



Agradecemos al Centro de Investigación y de Estudios Avanzados por el apoyo otorgado para la participación del plenarista.

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"Metalofármacos: Una Alternativa Terapéutica, Diseño, Actividad y Mecanismos de Acción"

Dra. Lena Ruiz Azuara
Facultad de Química, Departamento de Química Inorgánica y Nuclear, UNAM

Modera: Dra. María del Jesús Rosales Hoz. Departamento de Química, CINVESTAV.

Jueves 28 de septiembre Horario: 18:30-19:30 Salón: Rivera + Siqueiros

Semblanza

Obtuvo la Licenciatura en Química en la F.Q. de la UNAM, el Doctorado en Química (Q. Inorgánica) en la Universidad de Edimburgo (U.K), Posdoctorados en: la Universidad de Cambridge (UK), en la Universidad de Nuevo México, Las Cruces (U.S.A), Institut de Recherches Sur la Catalyse (Centre National de la Recherche Scientifique, Lyon, France). Actualmente es Profesor Titular C*, de la Facultad de Química de la UNAM. Catedrático Nivel 2*, PRIDE D*, SNI nivel III*. Áreas de investigación, Química Inorgánica, Química de Coordinación: Organometálica, Bioinorgánica, Química Inorgánica Medicinal, pionera de estas áreas en México. Fundadora y coordinadora de la Serie de conferencias "La Ciencia más allá del Aula" desde hace 17 años. Distinción por ser líder de área de la Royal Society of Chemistry como Fellow of the Royal Society of Chemistry, Premio Nacional de Química, Andrés Manuel del Río, 1998, entre otros reconocimientos internacionales y nacionales. Ha dirigido 49 tesis de Licenciatura 31 de Maestría y 17 de Doctorado. Su producción científica consta de 173 artículos de investigación de nivel Internacional y 13 nacionales; con más 3100 citas, 5 Artículos de Difusión, 27 Capítulos de libros, 40 Memorias en extenso, Patentes; 5 Internacionales y 2 Nacionales.

Resumen

En México existe una necesidad creciente por dar servicio a la demanda de salud en pacientes con cáncer. Entre los tratamientos útiles por su carácter sistémico se encuentra la quimioterapia; sin embargo, el costo de importación de estos tratamientos los hace inaccesibles a un gran número de pacientes. Por otra parte, la existencia de tumores refractarios a los quimioterapéuticos existentes, hace necesaria la búsqueda constante de nuevas opciones que permitan el desarrollo de agentes que superen las características de eficacia y costo de los tratamientos existentes.

En la Facultad de Química de la UNAM, nuestro grupo de investigación ha desarrollado una familia de compuestos de coordinación con centro metálico a base de metales esenciales, con actividad antineoplásica un grupo de moléculas han sido patentadas y Registradas con el Título de Marca Casiopeínas®. Las pruebas de evaluación in vitro e in vivo han cubierto los requisitos de actividad exigidos por los protocolos internacionales, tanto en modelos de isotransplantación como de xenotransplantación, demostrando efectividad y toxicidad moderada. Estas características aunadas a un bajo costo de producción en relación con otros quimioterapéuticos en el mercado, hacen a esta familia de compuestos una alternativa prometedora para el tratamiento de neoplasias malignas. Actualmente, uno de estos fármacos, la Casiopeina III-ia, se encuentra propuesto para su evaluación en Fase I. Los estudios de correlación estructura-actividad (QSAR) han apuntado a que 10 Casiopeínas son las potencialmente más activas dentro de las evaluadas.
Así mismo, se ha investigado el mecanismo de acción y se han identificado al menos dos blancos moleculares, la interacción directa con el ADN y la actividad nucleasa, la generación de especies reactivas de oxígeno, la muerte celular se ha determinado por las vías apoptóticas y autofágicas involucradas. La comprensión de esto último es fundamental para optimizar la actividad antitumoral de los compuestos mediante el diseño dirigido.
También se presentará en la conferencia, otras actividades presentadas por estos compuestos como antiparasitarios e hipoglucémicas. Así como otros sistemas químicos diferentes a las Casiopeínas con propiedades antiparasitarias importante.

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"Practical Direct Electrophilic Amination of Olefins and Aromatic Systems"

Prof. László Kürti
Department of Chemistry, Rice University

Modera: Dra. María del Jesús Rosales Hoz. Departamento de Química, CINVESTAV.
Viernes 29 de septiembre Horario: 9:30-10:30 Salón: Rivera + Siqueiros

Biosketch

László Kürti was born and raised in Hungary. He received his Ph.D. under the supervision of A.B. Smith at the University of Pennsylvania. There he authored the now popular textbook/reference book "Strategic Applications of Named Reactions in Organic Synthesis" with Barbara Czakó. Subsequently he was a Damon Runyon Cancer Fellow in the laboratory of E.J. Corey at Harvard University. László is now an Associate Professor of Chemistry at Rice University. The Kürti group focuses on the development of powerful new methods for the expedient enantioselective assembly of highly functionalized biaryls, heterocycles and carbocycles. László is the recipient of an NSF CAREER Award, Fellowship by the Japan Society for the Promotion of Science (JSPS), the 2014 Amgen Young Investigators' Award as well as the 2015 Biotage Young Principal Investigator Award.

Abstrac

Amines and their derivatives are ubiquitous substances since they make up the overwhelming majority of drug molecules, agrochemicals as well as many compounds that are produced by plants and living organisms (i.e., natural products). Aromatic amines appear as substructures in more than one third of drug candidates while aziridines, in which the nitrogen atom is bridged between two carbon atoms, are high-reactive and versatile building blocks for a large variety of functionalized amines. Not surprisingly, organic chemists spend a considerable amount of their time with the synthesis and late-stage functionalization of amines that serve as key chemical building blocks for the preparation of biologically active compounds, especially in medicinal chemistry. There is an urgent need for the development of novel carbon-nitrogen bond-forming methods and reagents that expand the toolbox of synthetic organic chemists and enable the environmentally friendly construction of complex molecular structures using the fewest number of chemical steps and generating the least amount waste.
A highly attractive, but currently underdeveloped, approach is the utilization of weak bonds as a driving force to achieve the rapid formation of much stronger bonds under mild conditions. The Kürti lab has been exploring several fundamentally new strategies for the transition-metal-free direct: (i) primary amination of arylmetals such as aryl Grignard reagents and arylboronic acids; (ii) intramolecular C(sp2)-H amination of arenes; (iii) double arylation of a suitable nitrogen linchpin reagents to afford N,N-diarylamines. We have also discovered, in collaboration with the Falck (UTSW) and Ess labs (BYU), the Rh-catalyzed direct N-H/N-alkyl aziridination of olefins as well as the primary (-NH2) and NH-alkyl amination of arenes, transformations that eluded synthetic chemists for decades. In-depth experimental and computational studies have already identified the critical factors required for efficient olefin NH- and N-alkyl aziridination as well as direct arene primary amination and led to the development of practical and chemoselective aminating agents.

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"Targeting DNA with Small Molecules for Imaging and Therapeutic Applications"

Prof. Ramón Vilar
Chair of Medicinal Inorganic Chemistry, Imperial College London

Modera: Modera: Dra. Lena Ruiz Azuara. Facultad de Química, UNAM

Viernes 29 de septiembre Horario: 19:00-20:00 Salón: Rivera + Siqueiros

Biosketch

Prof. Ramón Vilar holds since 2011 the chair of Medicinal Inorganic Chemistry at Imperial College London. He studied chemistry at the Universidad Nacional Autónoma de México (UNAM) followed by a PhD at the University of London (supervise by Prof Mingos). During this time his worked focused on organometallic chemistry of late transition metals. Between 1996 and 1998 he carried out postdoctoral studies in supramolecular chemistry at Imperial College London where he was later appointed as a Lecturer starting his independent career. In 2004 he moved to the Institute of Chemical Research of Catalonia (ICIQ) as an ICREA fellow and Group Leader, returning to Imperial College London in 2006. He held a prestigious EPSRC fellowship between 2009 and 2014. Over the past 15 years his research has mainly focused on the biological properties and medical applications of transition metals, with particular emphasis on the interaction of metal complexes and G-quadruplexes. He has published over 125 research papers, is inventor in 4 patents and has contributed to several books as author or editor.

Abstrac

DNA can assemble in a wide range of different topologies such as Z-DNA, triplexes and quadruplexes. With the mounting evidence that several of these non-canonical DNA structures play key biological roles, there is increasing interest in developing small molecules that can interact selectively with a given topology. In particular, over the past few years there has been increasing interest in the development of selective binders for guanine-quadruplexes (G-quadruplexes). G-quadruplex DNA has been shown to play important roles in regulation of gene expression, telomere maintenance and replication and therefore have been proposed to be attractive anticancer drug targets. This lecture will focus on the use of molecular tools to help us understand the biological roles of G-quadruplexes as well as their potential as drug targets.

Keywords: DNA, Quadruplexes, Bioinorganic, Imaging, Cancer

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Agradecemos a Facultad de Química de la Universidad Nacional Autónoma de México por el apoyo otorgado para la participación del plenarista.

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