

VII Workshop on Novel Methods for Electronic Structure Calculations

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Abstracts

Compositional and configurational optimisation of the electronic structure of energy materials

Ricardo Grau-Crespo

Department of Chemistry, University of Reading, Whiteknights Campus, Reading RG6 6AD, UK

The optimisation of materials for energy applications often relies on tuning their electronic structure to target a given functionality. For example, in photocatalytic semiconductors for hydrogen production via water splitting, the goal is to maximise light absorption from solar radiation while simultaneously achieving the correct band edge alignment with the relevant redox potentials, which leads to an ideal bandgap of around 2 eV. In thermoelectric semiconductors, a much narrower gap is required in order to achieve high electronic conductivity, while an asymmetry in the density of states about the Fermi helps increasing the thermopower. The most common approach in band structure engineering is to optimise a figure of merit in the composition space of a solid solution, which can be expensive to do experimentally. Density functional theory (DFT) calculations can provide useful guidance in solving this type of optimisation problem in a relatively inexpensive way, while also offering predictions on the stability of the proposed compounds. In this talk, I will present examples of recent research from my group where we have used DFT simulations to understand the thermodynamic stability and electronic structure of solid solutions with applications in energy devices. These include: i) shandite-structured mixed chalcogenides with promising thermoelectric behaviour [1]; ii) spinel-structured sulphides of interest as photovoltaic materials, where the bandgap can be tuned via changes in the degree of inversion of the cation distribution [2]; iii) metal organic frameworks where the band structure and alignment can be controlled via mixing of different metals or different linkers within the same structure [3,4].

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Materials Design in Practice: Atomistic Simulations in Science and Industry

Volker Eyert, Mikael Christensen, David Reith, Rene Windiks, Walter Wolf, Clive Freeman,
and Erich Wimmer

Materials Design SARL, 92120 Montrouge, France and Materials Design, Inc., San Diego, CA

During the past decades, atomic-scale simulations have emerged as an indispensable tool of materials research and engineering both in academia and industry. Leading industrial research laboratories, public laboratories, and universities have started to combine experimental data with the predictive power and the key to understanding materials properties as offered by atomistic simulations to solve engineering problems connected, e.g. to long-term stability of materials or to identify novel and environment friendly materials. In this situation, as the computer power is tremendously growing, comprehensive computational environments, which take away the burden of routine tasks, are coming to the fore, allowing researchers to focus on the scientific problem at hand. Using sophisticated model building and analysis tools the MedeA® software combines experimental structures and phase-diagrams with state-of-the-art computational procedures for property predictions for systems including alloys, semiconductors, ceramics, glasses, polymers, and fluids. Furthermore, the MedeA® software facilitates the simulation, e.g. of the electronic structure and mechanical properties as well as the thermal behaviour of complex structures such as interfaces, heterostructures, grain boundaries, defect structures and random alloys. The comprehensive capabilities of the MedeA® software will be illustrated by recent applications including the development of low-strain cathode materials for batteries, the analysis of grain-boundary stability in electronic devices, the electrical conductivity in alloys, and the search for optimum materials for hydrogen storage in the automotive industry.

Computational search and design of 2D materials and their Van der Waal heterostructures

Aldo H. Romero

Department of Physics and Astronomy, West Virginia University, Morgantown, WV-26505, USA

The traditional process of material design for a particular application was trial and error method, which did not only require large amount of resources but it was also very time consuming. The day-by-day enhancing power of computers and theoretical methods that describe the properties of materials has made us able to develop advanced computational methods that could predict the material properties with remarkable accuracy. In the first part of my talk, I will discuss one of such computational methods that we developed to perform structural search of 2D materials, which have recently come into much demand due to their numerous technological applications. Using this structural search method, one can efficiently explore the configurational space (potential energy surface) and search for the local minima of a given composition under the reduced dimensions. We employ a confining potential to restrict the movement of atoms during the optimization of the targeted energy function. We have applied this method and successfully predicted the lowest energy configuration of several materials in 2D. In the second part of my talk, I will present some of our recent results on various novel 2D systems that have promising applications in the spintronics technology. The major possible applications include the spin-field-effect transistors, detections for long-sought Majorana fermions, advanced sensors and optoelectronics devices.

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Electronic excitations in classical molecular-dynamics simulations

Eduardo Bringa (ebringa@yahoo.com)

CONICET and FCEN-UN Cuyo, Mendoza, Argentina

Interaction of radiation (photons or particles) with materials can lead to electronic excitations. Thermal spikes or two-temperature models can be successfully used to model coupling of electronic excitations to phonons, leading to phase transformations and defects. These models have been able to explain multiple experimental results, but their validity in nanostructures could be challenged. I will show examples of thermal spikes induced by ion bombardment in nanocrystalline diamond [1], silica [2], silica with embedded nanoparticles [3], and Au nanowires [4]. I will also show simulations of laser irradiation of gold nanofoams [5], where the electron-phonon coupling is varied to explore possible effects of coupling enhancement due to electron scattering in the nanostructure. In all cases, the simulations show permanent modifications which can be contrasted with experiments.

Future improved calculations of electron-phonon coupling and electronic excitations in nanostructures would lead to a better description of defects in irradiated materials, opening the possibility of tailoring certain modifications for technological applications, i.e. larger strength or ductility.

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Photocatalytic power of g-C₃N₄ and Ta₂O₅ for solar fuel production from first-principles calculations--quasi-particle theory and dispersive forces

Jorge M. Osorio-Guillén¹, William F. Espinosa-García¹, Santiago Pérez-Walton², Moyses Araujo³

¹Instituto de Física, Universidad de Antioquia

²Instituto Tecnológico Metropolitano ITM

³Department of Physics and Astronomy, Uppsala Universitet

Solar-based production of organic fuels (e.g. methanol) through the reduction of carbon dioxide (CO₂) had attracted great attention in the last decades. One of the challenges is to find Earth abundant materials that meet at the same time the properties of efficient sunlight absorption and suitable band edge potentials, facilitating photon-driven charge transfer reactions.

In this work, we have employed quasi-particle theory and time-dependent Density Functional Theory (DFT) to achieve fundamental understanding of the electronic structure and optical properties of two relevant photocatalysts, namely C₃N₄ in the graphitic structures (g-h-triazine and g-h-heptazine) and Ta₂O₅. The aim is to assess the photocatalytic power of these compounds and establish structure-properties relationships. The calculations have been carried out within the framework of semi-local and van der Waals (vdW) exchange-correlation functionals for DFT. The quasi-particle energies were calculated by the non-self-consistent GW approximation.

The calculated band gaps are 2.92 and 2.94 eV for g-h- triazine and g-h-heptazine [1,2], respectively, which are in good agreement with previous theoretical findings [3]. Our results show that graphitic g-h-triazine displays the band edge potentials at suitable positions for direct CO₂ reduction to formic acid with a catalytic power of about 1 eV. We have also carried out a thorough investigation of surface states of Ta₂O₅ assessing the band alignments for different non-polar low-index facets of the B-phase [3]. We have found that the conduction band lies between 2.68 and 3.2 eV from the vacuum level, depending on the orientation. These results provide the basis for further improvement of the materials properties for application as suitable photocatalyst.

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First principles study of ferroelectricity in (111)-epitaxially strained SrTiO₃

Sebastian E. Reyes-Lillo^(1,2,3), Karin M. Rabe⁽⁴⁾ and Jeffrey B. Neaton^(2,3,5)

(1) *Departamento de Ciencias Físicas, Universidad Andres Bello, Sazié 2212, Santiago 837-0136, Chile*

(2) *Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*

(3) *Department of Physics, University of California, Berkeley, California 94720 USA*

(4) *Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA*

(5) *Kavli Energy NanoSciences Institute at Berkeley, Berkeley, California, 94720 USA*

Strontium titanate (STO) is a prototypical ABO₃ perovskite with a wide range of technological properties such as ferroelectricity, photocatalysis, and superconductivity. The effect of squared (001) epitaxial strain on STO has been extensively studied theoretically and experimentally, and has been shown to enhanced the macroscopic ferroelectric polarization at both compressive and tensile strain. In this work, using a combination of first principles calculations and Landau phenomenological modeling, we explore the effect of hexagonal (111) epitaxial strain in the structural and dielectric properties of STO. We find that (111)-strain induces novel structural distortions that are not present in either bulk or (001)-strained STO, leading to potentially new coupling mechanisms with strain and magnetism. In contrast to the (001) case, (111)-STO display only ferroelectric and antiferrodistortive phases at tensile and compressive strain, respectively. The (111)-strain versus temperature phase diagram of STO reveals a room temperature ferroelectric phase with an out of plane polarization component and a large polarization of 50 $\mu\text{C}/\text{cm}^2$ at +4% tensile strain. We compute the macroscopic polarization, born effective charges and phonon modes as a function of (111)-strain and investigate the low-frequency dielectric response of the system.

Interaction of graphene nanostructures with water molecules: Anthropogenic Dark Earth (ADE)

Ana Maria Valencia and Marilia J. Caldas

Universidade de Sao Paulo

e-mail: valencia@if.usp.br

Understanding the interaction of carbon materials with various molecules is a topic of interest in order to appreciate their potential applications in various fields. As part of the interest in studying this interaction, we can include a recent direction of investigation towards understanding the role of carbon nanostructures in soil fertility, what is called Anthropogenic Dark Earth (ADE) or, “Terra Preta de Indio”. Which refers to highly fertile patches immersed in large unferile areas, mainly due to remains of black charcoal, and it has been connected [1] to the interaction of water with disordered, packed graphene nano-flakes (GNFs).

We study the interaction of water molecules with GNFs, through ab initio Density Functional Theory in the Perdew-Burke-Ernzenhof (PBE) approximation [2] including van-der-Waals (vdW) interactions [2], as implemented in the FHI-aims [3]. We have chosen hexagonal, armchair and zigzag terminated GNFs isolated and packed in double layers. The arm-chair termination is important since it does not induce strong border effects and as such allows one to simulate the effect of water adsorption on larger flakes, or on the surface layer of stacked structures. As expected, it is essential to include vdW interactions for the description of stacked flakes. We simulate different configurations, with one or four water molecules. From our results, in the case of interaction water-GNF surface vdW is a relevant interaction, while in the internal space of the bi-flakes we find a strong competition between the vdW flake-flake interactions and dipolar water-flake interactions. We find that the molecule is stably adsorbed on the GNF surface, however our main result is that, isolated or in clusters, if inserted inside

the biflake, water is expelled.

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Energetic of water desalination through subnanometer porous graphene

Walter Orellana

Universidad Andres Bello, Sazié 2212, Santiago, Chile

worellana@unab.cl

The increasing scarcity of fresh water in the world and the search for low-cost mechanisms for seawater desalination have attracted a lot of attention recently toward nanoporous graphene as the ultimate membrane material for selective molecular sieving and salt rejection. Recently, nanoporous graphene with pore size in the range of 0.5-1.0 nm created by oxygen plasma etching, have shown salt rejection rates of nearly 100% as well as water flux reaching tremendously high values of three molecules per picosecond. [1] However, the role of pore size and pore-edge chemical functionalization in the water-transport and salt-rejection processes is not clear enough. In this talk, using dispersion-corrected density functional theory calculations and *ab initio* molecular dynamic (MD) simulations, we study the energetic and diffusion of water molecules and hydrated ions (Na^+ , Cl^-) passing through subnanometer pores in graphene. Pores of about 0.8 nm in diameter passivated with H atoms (hydrogenated pore) and (O,H) atoms (hydroxylated pore) were considered. Our results show water fluxes at almost zero driving pressure of about one molecule every 3 picosecond for the hydroxylated pore, in close agreement with recent experiments. Whereas for the hydrogenated pore, no water molecules cross the pore during 6 ps of simulation time, suggesting a central role of the pore-edge oxygen atoms in increasing water flux. We also find that both pores are effective to block hydrated Na^+ and Cl^- ions with large energy barriers, ranging from 12 to 15 eV.[2] Thus, the large energy required by hydrated ions to cross the pores reflects the strong electric field that they exert on the surrounding water molecules and the difficulty to break the hydration shells.

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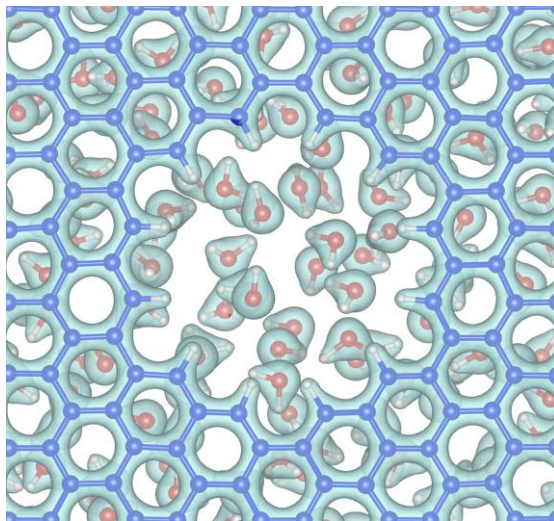


Figure 1: Hydrogenated pore of 0.8 nm in graphene

The thousand and one faces of the titania

Gabriela F. Cabeza
gcabeza@uns.edu.ar

GruMaSiCa, Grupo de Materiales y Sistemas Cataliticos
Depto. de Fisica, Universidad Nacional del Sur- IFISUR (CONICET-UNS)
Avda. Alem 1253, Bahia Blanca, Buenos Aires, Argentina

The titania (TiO_2) is a semiconductor and has its own name not only for its technological but also for its catalytic, including WGS reaction [1] and photocatalytic applications in its role as a photocatalyst in remedial reactions of environmental contaminants [2-3]. It has attracted interest in the study of possible modifications of it, in order to optimize the absorption of solar radiation by changing its wide band gap (BG), its potential redox and the half-life of charge carriers generated in the titania activation. Recently, experimental studies showed that monodoping with anions or cations have not reached the expected efficiency but it has been found that the mixed doping with transition metals and nonmetals greatly enhances the inhibition of recombination of charge carriers. Therefore, it is necessary to know accurately which ones are the contributions that each doping atom provides to the system. The accepted hypothesis is that the bands partially occupied close to the VB, resulting from the presence of nonmetal impurities, act as recombination centers (electrons of the partially occupied impurities states would annihilate the holes generated by the radiation absorbed) or as mobility reduction centers of charge carriers (the states of the metal impurities, near the CB, would immobilize the excited electrons) [4].

On the other hand, gas sensors based on TiO_2 films have been a subject of interest due to its high sensitivity and low cost. The sensing mechanism of this type of sensors is based on the conduction mechanism, which is governed by the potential barriers formed at the inter-grains of the polycrystalline structure. The shape of these potential barriers strongly depends on the characteristics of the material, and then it is expected that a doping aggregation will affect significantly the conductivity and thus the sensitivity of the sensor.

In this talk a careful theoretical analysis of the energetic, structural and electronic properties of doped and codoped titania [5, 6] and titania as metal support [7] will be presented with the aim to obtain insight into the metal-nonmetal effects as well as its applications in catalysis [8] and as a gas sensor [9]. Some of the results presented have been carried out in cooperation with experimental groups.

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Propiedades Vibratorias del Cu_3XY_4 (X=Nb,Ta y V: Y=S y Se) Mediante Dinámica Molecular Ab-Initio

Valencia Balvin- Instituto Tecnológico Metropolitano, Medellín, Colombia
Joaquín Peralta - Universidad Andrés Bello

En esta charla se explicará la caracterización de la Sulvanita cuyo fórmula química se encuentra dada por Cu_3XY_4 con X=Nb, Ta and V; Y= S, y Se. Este material es de gran interés debido a ser un potencial candidato para dispositivos de celdas solares y electrónicas de semiconductores transparentes. Se mostrará cómo a partir de cálculos de primeros principios se puede estudiar el comportamiento estructural y dinámico a diferentes temperaturas de la Sulvanita. Los resultados arrojados por este estudio utilizando la técnica de la teoría funcional de la densidad para temperaturas desde 300 K hasta aproximadamente 1500 K por medio de dinámica molecular ab-inicio en el ensamble microcanónico determina el espectro vibracional de esta familia de compuestos. Con esta información se mostrará la densidad parcial de estados vibracionales para diferentes temperaturas.

The state of iron at the interior of planets

Felipe Gonzalez

*Department of Earth and Planetary Science,
University of California, Berkeley*

The phase diagram of iron at high pressure is of considerable interest for geophysics and planetary science. The interior structure of rocky planets, such as the size and state of the core and related core-formation processes, depend on the detailed behavior of planetary materials, such as iron, at high pressure and temperature. Using density functional molecular dynamics, we investigate the melting curve of iron at megabar pressures. We derived the melting temperature by equating the Gibbs free energies of solid and liquid phases that we derived through the thermodynamic integration method. The melting curve allows us to study the crystallization behavior of iron under high compression. Our calculations show that the melting temperatures of iron are higher than extrapolations from previously calculated melting curves at lower pressures. Finally we compare its slope with the adiabatic gradient in order to determine how the cores of super-Earth planets crystallize.

Estructura Electrónica de los semiconductores $\text{Sn}_{1-x}\text{Ti}_x\text{O}_2$: Parametrización del potencial de intercambio TB-mBJ

A.V. Gil Rebaza¹, A.M. Mudarra Navarro¹, L. Errico^{1,2}, E.L. Peltzer y Blanca³

¹ *Instituto de Física La Plata IFLP-CONICET, Dpto. de Física de la Facultad de Ciencias Exactas de la Universidad Nacional de La Plata (UNLP), 1900 La Plata – Argentina.*

² *Universidad Nacional del Noroeste de la Provincia de Buenos Aires (UNNOBA), 2700 Pergamino –Argentina.*

³ *Grupo de Estudio de Materiales y Dispositivos Electrónicos (GEMyDE), Dpto. de Electrotecnia de la Facultad de Ingeniería, UNLP, 1900 La Plata – Argentina.*

Los óxidos de Sn y Ti (SnO_2 y TiO_2 , rutilo) han sido ampliamente estudiados debido a sus amplias aplicaciones tecnológicas en diversos dispositivos (como celdas solares, sensores de gas, dispositivos opto-electrónicos, entre otros), catálisis, fotocatalisis, etc. Estos compuestos, en la fase rutilo, experimentalmente poseen un band-gap directo de 3.6 eV y 3.3 eV, respectivamente. Recientemente, el sistema que se obtiene al combinar ambos óxidos, $\text{Sn}_{1-x}\text{Ti}_x\text{O}_2$, han sido propuesto como una alternativa para obtener semiconductores con un band-gap controlado, permitiendo aumentar la actividad de fotocatalisis y la sensibilidad de los sensores de gas.

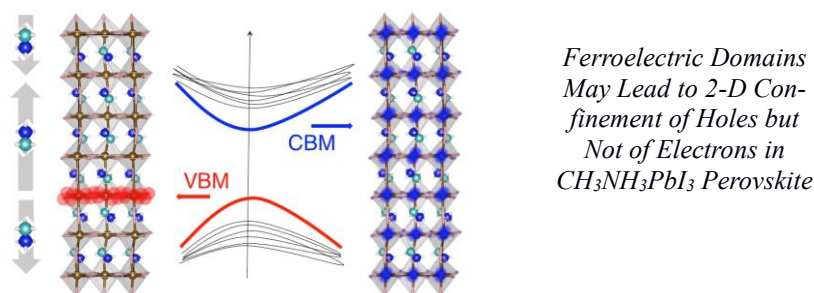
En el presente trabajo estudiamos, mediante un abordaje de primeros principios basado en la Teoría de la Funcional Densidad (DFT), las propiedades estructurales, electrónicas de los compuestos semiconductores $\text{Sn}_{1-x}\text{Ti}_x\text{O}_2$ ($0.0 \leq x \leq 1.0$) en función de la concentración de Ti (x). Con el fin de obtener una mejor descripción de la estructura electrónica (band-gap) de estos compuestos, se ha usado diferentes aproximaciones del potencial de intercambio-correlación, tales como GGA (PBE), meta-GGA y funcionales híbridas (HSE06). Se discutirá el caso meta-GGA del potencial de intercambio de Becke-Johnson modificado por Tran-Blaha (TB-mBJ). Analizaremos las diferentes parametrizaciones de dicho potencial y como varía el band-gap de los compuestos $\text{Sn}_{1-x}\text{Ti}_x\text{O}_2$. Se han usado el método Full Potential – Linearized Augmented Plane-Wave (FP-LAPW, Wien2k) como también el método de PseudoPotential Plane-Wave (PP-PW, Quantum Espresso), cuyos resultados se han comparado con datos experimentales obtenidos de la bibliografía.

Lattice distortions and polarizability effects in the behavior of photo-carriers of the metal-organic Perovskites

Ana L. Montero-Alejo,¹ E. Menéndez-Proupin,¹ P. Palacios,² P. Wahnón,³ J. C. Conesa⁴

¹Departamento de Física, Facultad de Ciencias, Universidad de Chile, Chile ²Instituto de Energía Solar and FyQATA, E.I. Aeronáutica y del Espacio, Universidad Politécnica de Madrid ³Instituto de Energía Solar and Dept. TFB, E.T.S.I. Telecomunicación, Universidad Politécnica de Madrid, Spain ⁴Instituto de Catálisis y Petroleoquímica, CSIC, Madrid, Spain.
Email: analilian.montero@gmail.com

Understanding the properties of the hybrid $\text{CH}_3\text{NH}_3\text{PbI}_3$ Perovskite is the cornerstone for advancing its applications in solar cell devices. It has been proposed the existence of separated diffusion paths for holes and electrons at the wall of ferroelectric nano-domains, generated by the local ordering of the organic cations. This could explain a reduction in the recombination of the charge carriers.^{1,2} We assess this idea from computational models and find that a two-dimensional hole confinement in $\text{CH}_3\text{NH}_3\text{PbI}_3$ is possible under room temperature conditions. However, our tetragonal phase models show that the alignment of dipole layers of organic cations induces the holes but not the confinement of electrons. This behavior does not change even by varying the strength of the ordered dipoles. The polarizable medium of Lead-Iodide ions deforms asymmetrically to shield the enclosed molecular dipole. The confinement of holes is favored by the distortions of the inorganic framework triggered by its interaction with the organic cations. Nevertheless, these lattice distortions counteract the effect of the oriented organic dipoles preventing the localization of the electrons.³ We highlight the importance of the inorganic framework polarizability as a guide of the carrier transport behavior in these materials.



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Harnessing the electronic structure of materials: from laser-induced robust states to crafted nonreciprocal bandstructures

Luis E. F. Foa Torres
FCFM, Universidad de Chile

Light-matter interaction is at the heart of intriguing phenomena and has led to many practical applications like, for instance, Raman spectroscopy. But beyond characterization, several studies have gone deeper into actually using light to modify the electrical properties of a material. This can be done, for example, by using light to switch off the conduction in graphene [1,2] (or other materials [3]), thereby allowing to tune the material's response with optical means, or even inducing tunable topological states in materials that would otherwise lack them [1,2,4,5,6,7,8] (i.e. a Floquet topological insulator [4]). In the first part of this talk I will present an overview on the electronic properties of materials/devices under strong laser irradiation.

In the second part of this talk I will focus on a different topic: achieving one-way transport by crafting a nonreciprocal bandstructure [9,10]. The ultimate case of this nonreciprocity is the realization of what is called an isolator, a system where transmission can occur only between say lead L and R and not viceversa while keeping a vanishing reflection at lead R.

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First principle predictions of hydrogen reservoirs. Lines of work at La Plata

Eitel L. Peltzer y Blancá

Group of Study of Materials and Electronic Devices (GEMyDE)

Dpto. de Electrotecnia, Facultad de Ingeniería. UNLP

The demand for clean energies grows rapidly, therefore, research into new materials to be used as hydrogen reservoirs are necessary. With this work we try to provide some understanding on simple and complex hydrides. The compounds studied are of the type L-H (where L is mainly Li) and Li-X-H, where X are, generally, lighter elements in the periodic table. With the participation of these elements we can obtain a high gravimetric hydrogen density. We performed a systematic study on these materials. In this work we used different ab-initio codes. The predictive power of first principle calculations have shown their importance in determining properties of new materials not yet synthesized. The ab-initio calculations help to shorten development times of new materials such as those proposed in this paper. Additionally, new data on materials studied in the past and others designed in this work are shown here. The second proposition is to show the lines of work in the group.