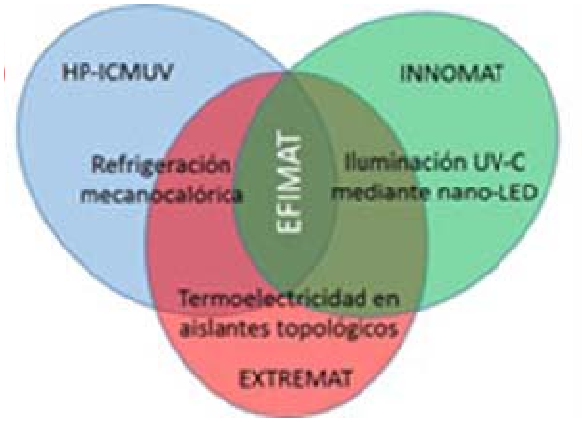
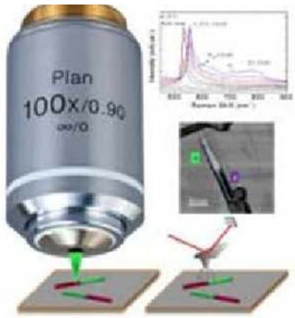
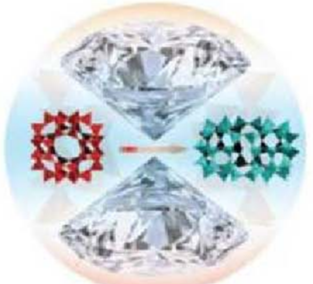
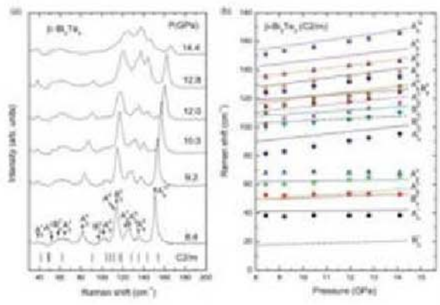


Program Book

SECOND EFIMAT WORKSHOP







GENERALITAT VALENCIANA
Proyecto EFIMAT
PROMETEO 2018 / 123

PARC CIENTÍFIC
UNIVERSITAT DE VALÈNCIA

ICMUV

Parc Científic de la Universitat de València

October 28 to 29, 2019

Introduction

EFIMAT is a research project supported by Generalitat Valenciana by means of a PROMETEO grant (Prometeo/2018/123 EFIMAT). This seeks to make a breakthrough in the use of energy through innovative but realistic proposals that take advantage of the synergy of three excellent research groups with complementary experiences. EFIMAT aims to develop advanced materials (LED-UV, materials with giant mechano-caloric effect, and thermoelectric materials based on topological insulators). The goal is to contribute to the development of efficient-energy applications highly demanded by industry and society, and which will allow our socio-economic environment to be at the vanguard of efficient-energy solutions. This second workshop covers almost all relevant research areas for EFIMAT and it is organized to boost the stimulating exchange of scientific ideas and results, creating new insights and collaborations.

Venue

The second edition of EFIMAT, Workshop for Advanced Materials for the efficient use of energy, will take place in Valencia October 28 and 29, 2019, at the Assembly Hall of the Edificio de Cabecera (first floor, University Research Institutes, Paterna).

Address: ICMUV. Catedrático José Beltrán 2. 46980 Paterna.

How to arrive: Visit https://efimat.blogs.uv.es/efimat/workshop2019/

General Schedule

October 28

Morning – Chairman: Juan Angel Sans

9:30 Opening Session – Ana Cros (ICMUV)

9:40 Alfonso San Miguel (Univ Lyon): Graphene and other 2D systems under high pressure: strain and doping effects

10:20 Francisco Javier Manjón (UPV): Metavalent bonding under pressure: the case of orpiment

11:00 Coffee Break

11:30 Nuria Garro (ICMUV): Epitaxial graphene intercalation: a route to doping control

12:10 Javier Ruiz-Fuertes (Univ. Cantabria): Structural solution of the high-pressure polymorph of scintillating β-$MgMoO_4$ by means of single crystal x-ray diffraction

12:50 Lunch Break

Afternoon – Chairman: Domingo Martinez-García

15:00 Robin Turnbull (Univ. of Edinburgh): An unusually complex phase of dense nitrogen at extreme conditions

15:40 Daniel Errandonea (ICMUV): Melting curve and phase diagram of vanadium and platinum under high-pressure and high-temperature conditions

16:20 Vesselin Donchev (Sofia Univ.): Investigation of dilute nitrides bulk layers and heterostructures for solar cells applications

October 29 – Chairman: Ana Cros

9:30 Alberto Otero de la Rosa (Univ. Oviedo): Challenges and new developments in the computational modeling of materials under pressure

10:10 Virginia Monteseguro (ICMUV): Unveiling the effect of the Pb 6s electronic levels in distinct $PbMoO_4$ under high pressure

10:50 Coffee Break

11:30 Albert Minj (IMEC, Leuven): Nanoscale investigation of (Al,Ga,In)N-heterostructures for optoelectronics and power applications

12:20 Enrico Bandiello (ICMUV): Phase transition of partially-hydrated $CePO_4$ under high-pressure conditions

13:00 Closing ceremony

Graphene and other 2D systems under high pressure: strain and doping effects

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Pressure is a three-dimensional concept and, as this, its application to low-dimensional systems leads to excursions out of the usual thermodynamic trajectories. To face such challenge requires the support of new paradigms related to membrane physics or even molecular physics. Here we will apply such concepts to the high pressure study of supported graphene or MoS_2 from the monolayer up to 3 layers. [1-5]

We will identify the different factors determining the pressure evolution of the system including the nature of the substrate and of the pressure transmitting medium or the bending rigidity of the 2D layer itself. Strain mismatch between layers or doping effects will be revealed through the study of isotopically labelled bilayer graphene (Fig 1) [5]. Opportunities on material design for energy applications will be also discussed [6].

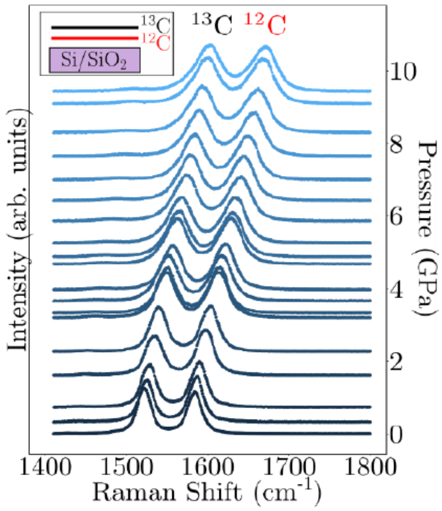

Fig. 1: Pressure evolution of the Raman spectrum of an isotopically labelled graphene bilayer sample. The inset shows the supported sample configuration.

[1] J. Nicolle et al., *Pressure mediated doping in graphene*, Nano Letters, 11, 3564 (2011)
[2] C. Bousige et al., *Biaxial strain in supported graphene*, Nano Letters, 17, 21 (2016)
[3] R.S. Alencar et al., *Atomic layered MoS_2 on SiO_2 under high pressure: bimodal adhesion and biaxial strain effects*, Physical Review Materials, 1, 024002 (2017)
[4] D. Machon et al., *Raman scattering studies of graphene under high pressure*, J. Raman Spectroscopy, 49, 121 (2018)
[5] A. Forestier et al, *Piezo-doping on bilayer graphene and mechanical layer decoupling*, Submitted (2019)
[6] D. Machon et al., *Perspective: High pressure transformation in nanomateirals and opportunities in material design.* J. App. Phys. 124 160902 (2018)

Metavalent bonding under pressure: the case of orpiment

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E. Lora da Silva,[1] C. Popescu,[4] J. Ibañez,[5] R. Vilaplana,[2] and F. J. Manjón[1,*]

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Metavalent or resonant bonding is a recently proposed new class of bonding that is intermediate between p-type covalent bonding and metallic bonding. It characterizes a new family of materials known as “incipient metals” [1]. Metavalent bonding occurs in materials where there is a deficiency of valence electrons in the unit cell to form a large number of bonds, such as in octahedrally-coordinated rocksalt-related structures occurring in GeTe, SnTe, PbSe, PbTe, Sb_2Te_3, Bi_2Te_3, Bi_2Se_3, Sb, Bi and $AgSb_2Te_4$.

The main characteristics of metavalent bonding are: i) a much higher cation coordination than that assumed with the 8-N rule; ii) very high Born effective charge and optical dielectric constant as compared to typical covalent materials; iii) high mode Grüneisen parameters of phonons and low wavenumbers of optical phonons as compared to typical covalent materials; and iv) a moderately high electrical conductivity caused by the small bandgap which stems from the partial delocalization of electrons between several bonds.

Arsenic sulfide (As_2S_3), and in particular the monoclinic polymorph (α-As_2S_3), aka orpiment, is one of the ores of As together with realgar (α-As_4S_4) and arsenopyrite (FeAsS) minerals [2]. In particular, orpiment and realgar are known since ancient times, where realgar was used as a red pigment and orpiment as a gold- like pigment (*Aurum pigmentum* in latin), hence his mineral name orpiment [3].

Despite existing several high-pressure studies on orpiment [4], many of its properties are not well known even at ambient pressure. In particular, the behavior of its structural, vibrational and electronic properties both at room and high pressure are far from being understood. Here, we present a joint experimental and theoretical study of the structural, vibrational and electronic properties of orpiment under compression, which unveils the internal mechanisms that emerge in orpiment during compression. We discuss the equation of state and the internal polyhedral compressibility, the symmetry and behavior of the Raman-active modes and the of the electronic band structure of orpiment under compression and compare them to its parent binary compounds.

Our XRD and Raman measurements together with theoretical calculations evidence the presence of an isostructural phase transition around 25 GPa leading from a three-fold coordination of As atoms at room pressure to an As coordination larger than five above 25 GPa (see Fig. 1).

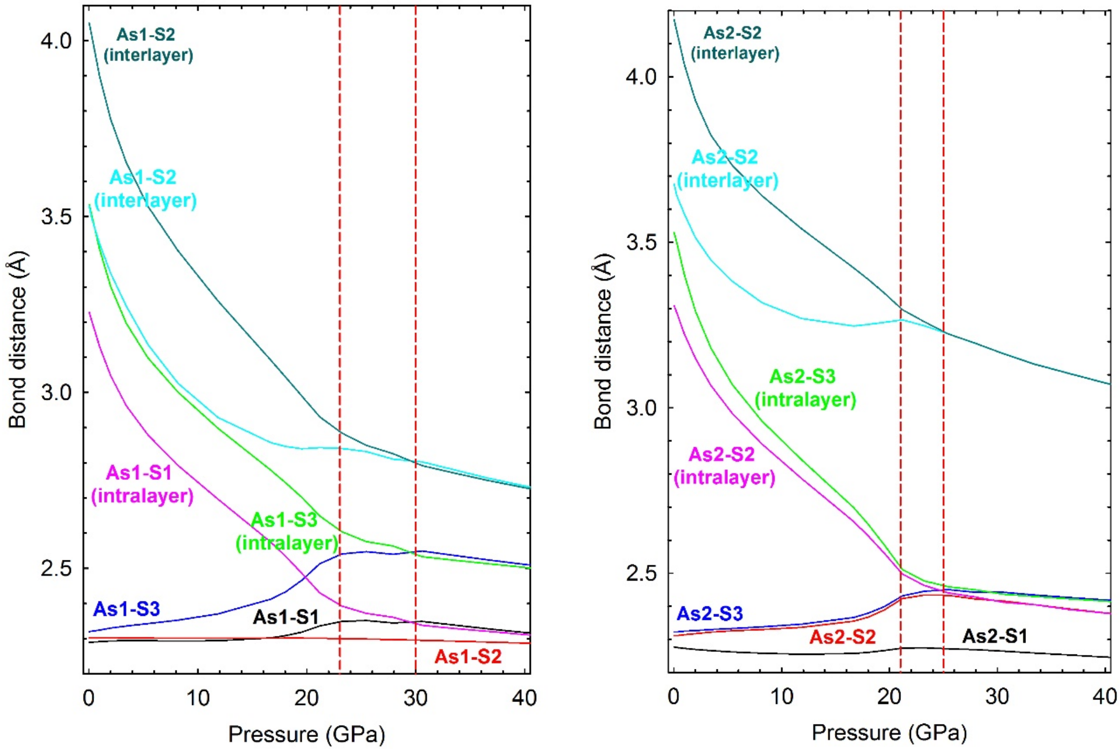

Fig. 1. Theoretical pressure dependence of the interatomic distances in orpiment with (solid) and without (dashed) van der Waals interactions.

The behavior of the structural parameters, Raman and infrared vibrational frequencies and optical bandgap of orpiment under compression can be understood on the light of the metavalent bonding concept; i.e. above 25 GPa, orpiment undergoes a transition from a solid featuring intra-layer p-type covalent bonds and inter- layer van der Waals bonds to a solid with intra-layer and partially inter-layer resonant bonds. This behavior is similar to that recently found for GeSe, where a pressure- induced intra-layer metavalent bonding is observed above 40 GPa after a first-order phase transition [5]. On further compression, full metallization of orpiment is predicted, which is observed above 40 GPa.

In summary, pressure transforms orpiment, a layered semiconductor with p-type covalent bonds and van der Waals interactions at room pressure, into an incipient metal, with metavalent bonds, above 25 GPa, and finally into a metal, with metallic bonds, above 40 GPa. We propose that this path from covalent bonding to metal bonding going through metavalent bonding is also followed by many other compounds with IV-VI and V_2- VI_3 stoichiometry as well as by their related ternary and multinary compounds.

[1] M. Wuttig et al. Adv. Mat. 2018, 30, 1803777.

[2] J. D. Smith et al. The Chemistry of Arsenic, Antimony and Bismuth, Pergamon Texts in Inorganic Chemistry (Pergamon Press, 1973).

[3] Pliny the Elder, Naturalis Historia, Chapter 22 (Taylor and Francis, London, 1855).

[4] K. X. Liu et al. Materials 2019, 12, 784. [5] M. Xu et al. J. Phys. Chem. C 2017, 121, 25447.

Epitaxial graphene intercalation: a route to doping control

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In this work we study epitaxial graphene on (0001) SiC before and after being exposed to several plasmas in the ultra-high vacuum chamber of an MBE system. We report on the formation of a self-limited Ga or In metallic bilayer which gets intercalated between graphene and the SiC surface by diffusion at SiC steps. The role of N and Ga deposition on the characteristics of graphene are investigated in different samples. The structural changes under the different treatments are addressed by Atomic Force Microscopy (AFM), and correlated with the electrical properties of the 2D layer by Kelvin Probe Force Microscopy (KPFM). Strain and doping of the graphene layers were extracted from Raman scattering maps. The results obtained indicate that the intercalation of N or metal species between graphene and SiC takes place only in one-layer graphene regions, leading to the full decoupling of graphene from the SiC surface. When effectively detached from SiC, graphene decreases its doping level and improves considerably both strain and doping homogeneity.

Structural solution of the high-pressure polymorph of scintillating β-MgMoO$_4$ by means of single crystal x-ray diffraction

J. Ruiz-Fuertes[1,*], A. Friedrich[2], N. Garg[3], D. Errandonea[4], P. Rodríguez-Hernández[5], and A. Muñoz[5]

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Ionizing radiation and particle physics scintillating detectors, tunable lasers, or optoelectronic devices are some of the applications in which monoclinic molybdates and wolframates can be found. The reason is their high light yield emission when hit by γ-particles or x-rays. Unfortunately, their emission shows long scintillation times that range from 12−15 μs. This drawback has been tried to be palliated up to some extent by the tune of the optical properties of molybdates using high pressure or high temperature. However, these scintillating compounds present a vast polymorphism at extreme conditions. CdWO$_4$ presents a bandgap collapse of 0.5 eV at 21 GPa as a consequence of a structural phase transition from a wolframite-type structure to an unknown structure which cannot be understood considering a phase transition to a phase consisting of two coexisting structures [1]. β-MgMoO$_4$ crystallizes in a monoclinic structure (C2/m) and undergoes a phase transition to an irreversible and unknown structure at 1.4 GPa [2]. According to a previous Raman spectroscopy study this pressure-induced phase transition involves a coordination increase from 4 to 6 of the MoO$_n$ polyhedra and involves either no change of the symmetry elements of the crystal or the loss of the centering of the unit-cell. Here we focus on the structural solution of the high-pressure phases of CdWO$_4$ and β-MgMoO$_4$ by means of synchrotron single-crystal x-ray diffraction experiments. Our studies unveil for CdWO$_4$ a $P2/c \rightarrow P2_1/c$ phase transition involving a doubling of the unit cell and for β-MgMoO$_4$ an isosymmetric phase transition in which the Mo polyhedra increase their coordination from tetrahedral to octahedral with half of the Mg and Mo polyhedra aligning two of their distances along the [001] direction.

[1] R. Lacomba-Perales, D. Errandonea, D. Martinez-Garcia, P. Rodríguez-Hernández, S. Radescu, A. Mujica, A. Muñoz, J. C. Chervin, and A. Polian, Phys. Rev. B 79, 094105 (2009).

[2] M. N. Coelho, P. T. C. Freire, M. Maczca, C. Luz-Lima, G. D. Saraiva, W. Paraguassu, A. G. Souza Filho, and P. S. Pizani, Vibrational Spectroscopy 68, 34 (2013).

An unusually complex phase of dense nitrogen at extreme conditions

Robin Turnbull[1,*], Michael Hanfland[2], Jack Binns[3], Miguel Martinez-Canales[1],
Mungo Frost[1,4], Miriam Marqués[1], Ross T. Howie[3] and Eugene Gregoryanz[5,3,1]

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[3]*Center for High Pressure Science & Technology Advanced Research, Shanghai, China.*

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Nitrogen exhibits an exceptional polymorphism under extreme conditions, making it unique amongst the elemental diatomics and a valuable testing system for experiment-theory comparison. Consequently, the pressure-temperature (P-T) phase diagram of nitrogen (shown in Fig. 1) has been a focus-point in high pressure research for the past 20 years. Despite attracting considerable attention [1-3 and refs. therein], the structures of many high-pressure nitrogen phases still require unambiguous determination. This presentation will focus on contemporary exploratory work into the nitrogen P-T phase diagram, with an emphasis on experimental techniques and the elusive high-pressure high-temperature polymorph ι–N_2 (pronounced 'iota'–N_2), the structure of which was recently revealed for the first time [3].

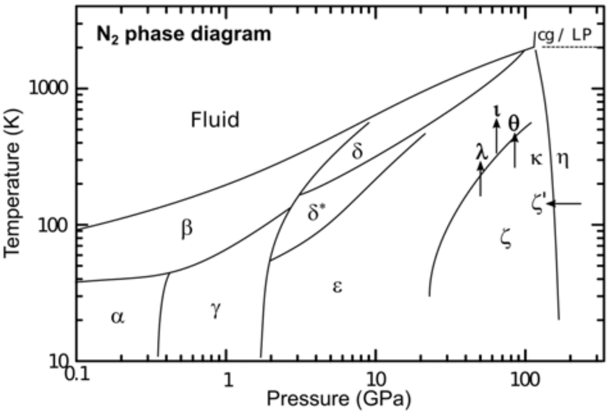

Fig. 1: The pressure-temperature phase diagram of elemental nitrogen.

[1] Gregoryanz, E., *et al.* Raman, infrared, and x-ray evidence for new phases of nitrogen at high pressures and temperatures. *Phys. Rev. B* 66, 224108 (2002).

[2] Frost, M., *et al.* E. Novel high-pressure nitrogen phase formed by compression at low temperature. *Phys. Rev. B* 93, 024113 (2016).

[3] Turnbull, R., *et al.* Unusually complex phase of dense nitrogen at extreme conditions. *Nat. Commun.* 9, 4717 (2018).

Melting curve and phase diagram of vanadium and platinum under high-pressure and high-temperature conditions

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Recent published results on the melting curve and phase diagram of vanadium (V) and platinum (Pt) under high-pressure and high-temperature conditions will be presented and discussed. The reported investigation includes a combination of experimental and theoretical studies of the melting curve and the structural behavior under extreme pressure and temperature. We performed powder x-ray-diffraction experiments up to 120 GPa and 4800 K, determining the phase boundary of the body-centered cubic-to-rhombohedral transition in V and the melting temperatures at different pressures for Pt and V. Melting temperatures have also been established from alternative methods and from density-functional theory calculations. Results obtained from our experiments and calculations are fully consistent and lead to an accurate determination of the melting curve of V and Pt. These results are discussed in comparison with previous studies including shockwave experiments. Finally, a high-pressure, high-temperature equation of state for the two studied metals will be discussed.

[1] S. Anzellini, V. Monteseguro, E. Bandiello, A. Dewaele, L. Burakovsky, and D, Errandonea, Scientific Reports 9, 13034 (2019).

[2] D. Errandonea, S. G. MacLeod, L. Burakovsky, D. Santamaria-Perez, J. E. Proctor, H. Cynn, and M. Mezouar, Phys. Rev. B 100, 094111 (2019).

Investigation of dilute nitrides bulk layers and heterostructures for solar cells application

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Dilute nitrides (such as InGaAs(Sb)N, GaAsSbN) form a novel class of semiconductor alloys, which has emerged from the conventional III-V compounds by incorporating a small amount of nitrogen. The interest in these compounds is due to their potential to alter the energy band gap and the lattice constant, which creates additional flexibility desired in many applications such as multijunction solar cells[1], heterojunction bipolar transistors [2] and high-speed photodetectors [3] .

GaAsSbN layers and structures are grown by low-temperature liquid-phase epitaxy (LPE) on GaAs substrates and are characterized in view of the application of this material in solar cells. The GaAsSbN layers exhibit reproducible properties and good optical quality. A number of experimental methods including X-ray diffraction, energy dispersive X-ray spectroscopy, atomic force microscopy, X-ray photoelectron spectroscopy (XPS) and Raman spectroscopy are applied for investigation of the structural properties, surface morphology, local arrangement and chemical bonding of Sb and N in the obtained compounds. XPS spectra reveal clearly the Sb content and give indication for the presence of N (around 0.1 at.%) [4]. The band gap values at room temperature assessed from surface photovoltage (SPV) and photoluminescence (PL) measurements are in good agreement. They are 20-30 meV lower than those of reference GaAsSb layers and around 190-230 meV lower than the band gap of GaAs. PL spectra measured at different temperatures (10 - 300K) show a very weak S-shape-like behaviour of the PL peak energy position indicating minimal carrier localization. Electrical measurements have demonstrated that Mg is suitable dopant for obtaining from closely compensated to highly doped p-type GaAsSbN layers. Based on this result GaAs/GaAsSbN/GaAs p-i-n heterostructures, based on closely compensated GaAsSbN are grown for the first time by the LPE method. PL and SPV measurements reveal good optical quality of the structures with low concentration of localized states and photosensitivity red limit extended in comparison to GaAs down to about 1.2-1.24 eV.

The obtained results can be used as a base for further development of the LPE technology for fabrication of solar cells based on GaAsSbN material.

[1] Aho A, Isoaho R, Hytönen L, Aho T, Raappana M, Polojärvi V, Tukiainen A, Reuna J, Mäkelä S and Guina M. *Lattice-matched four-junction tandem solar cell including two dilute nitride bottom junctions.* Prog. Photovoltaics Res. Ap*pl.* (299– 305), **27,** (2019).

[2] Asbeck P M, Welty R J, Tu C W, Xin H P and Welser R E. *Heterojunction bipolar transistors implemented with GaInNAs materials. S*emicond. Sci. Technol. (898–906), **17**, (2002).

[3] Chen W C, Su Y K, Chuang R W, Yu H C, Chen B Y and Hsu S H. *Investigation of InGaAsN MSM photodetectors with transparent ITO Schottky contacts*. Semicond. Sci. Technol. (035027), **23,** (2008).

[4] Milanova M, Donchev V, Kostov K L, Alonso-Álvarez D, Terziyska P, Avdeev G, Valcheva E, Kirilov K and Georgiev S. *Study of GaAsSb:N bulk layers grown by liquid phase epitaxy for solar cells application.s* Mater. Res. Express (075521), **6**, (2019).

Challenges and new developments in the computational modeling of materials under pressure

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In this talk, I will present some of the recent developments in the field of computational modeling of materials behavior under extreme pressure and temperature conditions. Three separate topics will be covered: 1) The emerging challenge of molecular phase diagram prediction, i.e., the calculation of the stable solid-state phase of a molecular compound from the sole knowledge of its molecular diagram; 2) the difficulties of common density-functional theory methods in modeling seemingly simple systems like Au_2S and Ag_2S, related to shortcomings of the density functionals used in periodic solids; and 3) a new computational method for the calculation of delocalization indices between atoms and molecules in solids and its application to track bonding in simple molecular crystals under high pressure.

Unveiling the effect of the Pb 6*s* electronic levels in distinct $PbMoO_4$ under high pressure

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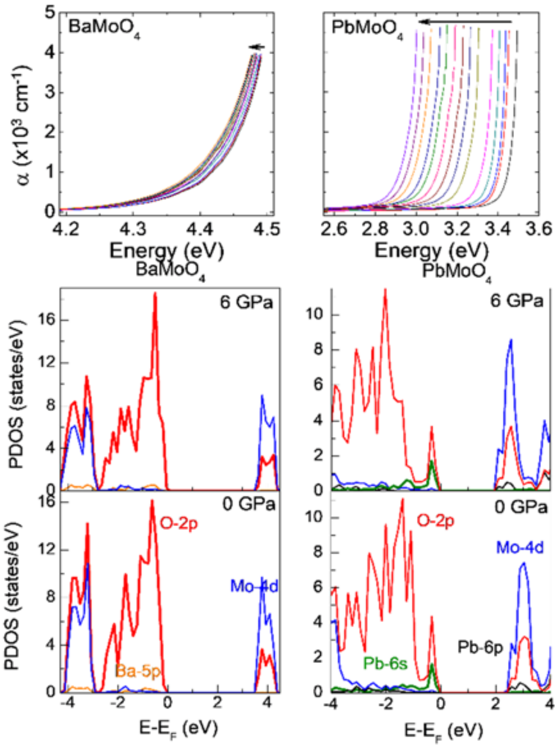
Lead molybdate ($PbMoO_4$) belongs to a family of scintillating crystals in which the understanding of the nature of their bandgaps is crucial to tune their luminescent properties. However, questions as why $PbMoO_4$ has a direct bandgap extremely sensitive to compression (-50 meV/GPa), why its location is at ∑, away from zone center and why it is considerably narrower than its scheelite-type counterparts, remain unsolved. [1, 2] In this work, we employ optical absorption spectroscopy, *ab initio* electronic band structure and electronic localization function calculations under high pressure to unveil, for the first time since 1985, the real origin of the bandgap of $PbMoO_4$. Moreover, we determine the exact bandgap value of $PbMoO_4$, $BaMoO_4$, and $CdMoO_4$ which requires a fit to Urbach's law.



[1] Y. Zhang, N. A. W. Holzwarth, and R. T. Williams, *Physical Review B* 1998, 57, 12738.

[2] A. Jayaraman, B. Batlogg, and L. G. VanUitert, *Physical Review B* 1985, 31, 5423.

Nanoscale investigation of (Al,Ga,In)N-heterostructures for optoelectronics and power applications

Albert Minj[1, 2*], Ana Cros[3], Nuria Garro[3]

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Wide band gap Gallium nitride-based semiconductors with extremely favorable thermal and electrical properties are confidently penetrating power conversion and optoelectronics market [1, 2] by accommodating large number of applications covering light-emitting to high power electronic devices, which are a necessity for the next generation of automobiles and home appliances. This is because of the important technical advantages III-nitrides has to offer, including high tunability of direct band gap from ultra-violet to infra-red energies, anisotropic polarization, 10× higher breakdown strength than Si, faster switching speed, higher thermal conductivity and so on, which brings up the possibility of producing highly efficient monolithic solid-state colour-mixed light-emitting diodes and of pushing up frequencies of power electronics system beyond the capacity of traditional silicon counterparts. Despite their high potential, there remains main challenges related to incomplete understanding of strain relaxation phenomena and surface defects in these materials and therefore, scientific focus on nanometer scale studies combining electrical and chemical analysis are of paramount importance. To address these issues, a combinational approach of multiple scanning probe microscopy methodologies, Conductive-Atomic force microscopy, Scanning capacitance microscopy and Kelvin probe force microscopy, sensitive to free carriers, charges and potential in the III-nitride heterostructures is employed. A special emphasis is given on photo-assisted Kelvin probe force Microscopy for investigation of surface states and extended defects, which takes advantage of direct access to local surface photovoltage formed via illumination (visible-to-UV) of sample in response to electron excitation via defect levels and band edge absorption.

[1] *Power GaN 2017: epitaxy, devices, applications, and technology trends 2017*. Market & Technology report - October 2017

[2] Ren, F. and Zolper, J.C. *Wide Band Gap Electronic Devices*. World Scientific: Singapore, 2003

Phase transition of partially-hydrated CePO$_4$ under high-pressure conditions

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CePO$_4$ is a dimorphic material with multiple potential applications, among which energy storage devices [1] and sensors for O$_2$, Fe^{2+}, Co^{2+} and glucose [2–6]. At ambient conditions it crystallizes in both a monoclinic monazite (S.G. $P2_1/n$) and a hexagonal structure (S.G. $P6_222$) [7]. The latter polymorph mainly exists in the hydrated CePO$_4$·xH$_2$O form, being water necessary for its stabilization. The stability of the hexagonal polymorph has thus been mainly the concern of high-temperature studies, which have shown that upon annealing and water removal, hexagonal CePO$_4$ indeed collapses to the monazite structure [8,9]. Monazite CePO$_4$, has also been shown to be stable in high-pressure conditions up to at least 30 GPa [10,11] while there is a complete lack of high-pressure studies on hexagonal CePO$_4$.

The behaviour of the hexagonal polymorph under high-pressure conditions, up to 21 GPa, is presented here. A second-order phase transition to a novel polymorph is detected at a pressure of 10 GPa for hexagonal, partially-hydrated CePO$_4$. This previously unreported high-pressure phase has a monoclinic structure with an atomic arrangement similar to that of the low-pressure phase, but with reduced symmetry, and belongs to monoclinic $C2$ space group. There is no detectable volume discontinuity at the phase transition (Figure 1).

Here we provide structural information on the new phase and determine the axial compressibility and bulk modulus for both phases. The compressibility is found to be anisotropic for both polymorphs and their bulk moduli is about 2/3 of that of the denser monazite phase.

In addition, the isothermal compressibility tensor for the high-pressure structure is reported at 10 GPa and the direction of maximum compressibility is calculated. The possible role of water and of the pressure medium in the high-pressure behaviour is also discussed.

[1] P. Pusztai, H. Haspel, I. Y. Tóth, E. Tombácz, K. László, Á. Kukovecz, Z. Kónya, ACS Appl. Mater. Interfaces 2015, 7, 9947.

[2] M. Kirubanithy, A. A. Irudayaraj, A. D. Raj, S. Manikandan, Mater. Today Proc. 2015, 2, 4344.

[3] W. Di, X. Wang, X. Ren, Nanotechnology 2010, 21.

[4] H. Chen, J. Ren, Analyst 2012, 137, 1899.

[5] H. Chen, F. Yuan, J. Xu, Y. Zhang, Y. Wu, L. Wang, Spectrochim. Acta - Part A Mol. Biomol. Spectrosc. 2013, 107, 151.

[6] G. Yan, Y. Zhang, W. Di, W. Qin, Dye. Pigment. 2018, 159, 28.

[7] R. C. L. Mooney, Acta Crystallogr. 1950, 3, 337.

[8] P. Pusztai, T. Simon, Á. Kukovecz, Z. Kónya, J. Mol. Struct. 2013, 1044, 94.

[9] L. Bo, S. Liya, L. Xiaozhen, W. Tianmin, K. Ishii, Y. Sasaki, Y. Kashiwaya, H. Takahashi, T. Shibayama, J. Mater. Sci. Lett. 2000, 19, 343.

[10] T. Huang, J. S. Lee, J. Kung, C. M. Lin, Solid State Commun. 2010, 150, 1845.

[11] D. Errandonea, O. Gomis, P. Rodríguez-Hernández, A. Muñoz, J. Ruiz-Fuertes, M. Gupta, S. N. Achary, A. Hirsch, F. J. Manjon, L. Peters, G. Roth, A. K. Tyagi, M. Bettinelli, J. Phys. Condens. Matter 2018, 30, 06540.