



Science Meeting – Scientific Report

The scientific report (WORD or PDF file - maximum of seven A4 pages) should be submitted online within two months of the event. It will be published on the ESF website.

Proposal Title: *Workshop on advanced ab-initio simulations of materials under extreme pressure conditions*

Application Reference N°: *5252*

1) Summary (up to one page)

In the framework of the 52nd European High Pressure Research Group (EHPRG) International Meeting held in Lyon, France from 7 to 12 september 2014 we organized a one day workshop focused on the use of advanced ab-initio simulations of materials under extreme conditions.

The 52nd EHPRG gathered 235 participants of the European high pressure community of physics, chemistry, geosciences, engineering and other fields as food processing, biosciences or medical applications.

The 52nd EHPRG Meeting was coupled with the UNESCO International Year of Crystallography and special sessions on Crystallography under extreme conditions were also organized. It is without saying the importance of the coupling of advanced crystallographic techniques with state-of-the-art predictive tools to explore the possibilities of synthesis of new materials or to refine models of the Earth interior as well as the composition of other planets.

The International Scientific Advisory Committee of the EHPRG has been chosen to participate together with the organizers to the selection of invited and oral contributions. The SAC constituted of 26 members counted with 4 theoreticians which together with the two chairs of the ab-initio advanced workshop were charged on the program organization.

2) Description of the scientific content of and discussions at the event (up to four pages)

Materials and molecules under high pressure constitute an excellent benchmark to test the predictive capabilities of ab-initio simulations and it has strongly contributed to the development of DFT.

This workshop, consisting on 1 plenary session, two parallel sessions and a poster session was chaired by M. Marques and R. Caracas, members of the Organizing Committee of the 52nd EHPRG. *All sessions of the workshop were open to all participants to the EHPRG Conference.*

Prof. Yanming MA, Univ. Jilin, China was the plenary speaker and presented the advances of particle swarm method for structure prediction. He showed how the prediction of atomistic structures with the given information of chemical compositions at chosen pressure conditions becomes crucially important. However, it is an extremely difficult as it basically involves classifying a huge number of energy minima on the energy surface. He presented the CALYPSO approach for structure prediction based on the particle swarm optimization algorithm, describing how the method takes the advantage of swarm intelligence and smart learning. After giving a short introduction into the principle of CALYPSO structure prediction method he showed applications into the exploration of novel high-pressure structures. Examples of the exotic physics and chemistry not accessible at ambient pressure were revealed. Examples included the prediction and its later experimental confirmation of insulating electride lithium, out-of-imagination cage structure of polymeric nitrogen or spiral chain form of oxygen. Unexpected chemical reactions of Fe and Xe, and Ca and H₂ at extreme conditions with the formation of unusual stoichiometries were also reported. Reaction of Fe and Xe in the conditions of Earth core might provide a possible solution of the “missing Xe paradox”

In the corresponding oral sessions and poster session, there was presented a high variety of modelization of the electronic interactions in high pressure systems. An important part of the contributions referred to structural prediction and their consequences on the thermodynamic properties (bulk modulus, sound velocity), electronic state (and transitions between insulator and metallic states) or, magnetic properties, between others.

3) Assessment of the results and impact of the event on the future directions of the field (up to two pages)

One main conclusion was the recognized capabilities of the present structural prediction methods which can now guide experiments on the realization of new unknown phases. The effect of temperature appears as the most challenging in order to apply such methods to planetary conditions in particular.

4) Annexes

4a) Programme of the meeting

4b) Final Budget

4c) Full list of speakers and participants

Annex 4a: Programme of the meeting

One plenary talk

Plenary 4 FRIDAY	ROOM: Auditorium Malraux Chair: J.M. Recio
09:00- 10:00	Exploring Novel Physics and Chemistry at Extreme Conditions: A Leading Role of Swarm-Structure prediction <u>Yanming MA</u>

Two parallel sessions

Session 18 WEDNESDAY	Theory 1 ROOM : 3 Chair: A. Muñoz
10:30- 10:50	Computational evidence of a silicon carbonate structure stable at high pressure <u>A. Morales-Garcia</u> , M. Marqués, J. M. Menéndez, V. G. Baonza, J. M. Recio
10:50- 11:10	Compressibility of carbonated glasses <u>Razvan Caracas</u>
11:10- 11:30	Electronic, elastic and vibrational properties of yttrium aluminium garnet under high pressure from ab initio studies <u>V. Monteseuro</u> , P. Rodriguez-Hernandez, F. J. Manjon, V. Lavin and A. Munoz
11:30- 11:50	Pressure dependence of binary phase diagrams from sound velocity measurements M.Emuna, Y. Greenberg, E.Yahel, <u>G. Makov</u>

Session 20 THURSDAY	Theory 2 ROOM : 2 Chair: Y. Ma
13:30- 14:00 Invited	Progress in theoretical description of pressure induced phase transitions <u>I. A. Abrikosov</u> , M. Ekholm, Q. Feng, J. M. Wills, I. Yu. Mosyagin, L.V. Pourovskii, L. Dubrovinsky
14:00- 14:20	Quantum-driven phase transition in high-pressure ice <u>Yael Bronstein</u> , Philippe Depondt, Fabio Finocchi, Antonino Marco Saitta
14:20- 14:40	Ab-initio Thermodynamics of High Pressure phases of polymeric Nitrogen <u>S.Uma Maheswari</u> , Karsten Albe
14:40- 15:00	Understanding phonon-driven superconductivity in group-IV layered superconductors in a single electronic picture <u>Jose A. Flores Livas</u> , Antonio Sanna

One poster session

Theory and Modelling	
P95	Thermodynamic properties of titanium group metals from ab-initio calculations <u>Uri Argaman</u> , Eitan Eidelstein, Ohad Levy, Guy Makov
P96	Influence of pressure on phase stability of binary and multicomponent alloys <u>S. A. Barannikova</u> , A. M. Zharmukhambetova, A. Yu. Nikonov, A. V. Dmitriev, A. V. Ponomareva, I. A. Abrikosov
P97	Theoretical investigation of the collapse of single, double and triple wall carbon nanotubes under hydrostatic pressure <u>T.F.T. Cerqueira</u> , S. Botti, A. San-Miguel, M.A.L. Marques
P98	High-pressure behavior of electron structure and electronic transport properties of europium <u>V.V. Gapontsev</u> , N. V. Morozova, S. V. Ovsyannikov, V. V. Shchennikov
P99	Review on distorted face-centered cubic phase in yttrium via genetic algorithm <u>T. Ishikawa</u> , T. Oda, N. Suzuki, K. Shimizu
P100	Guest-Host Interactions in Gas Clathrates Hydrates Under Pressure <u>F. Izquierdo-Ruiz</u> , A. Otero-de-la-Roza, J. Contreras-Garcia, J. M. Menendez, O. Prieto-Ballesteros, J. M. Recio
P101	Tetrahedral polymorphs of Silicon obtained by structure searching <u>A. Mujica</u> , C. J. Pickard, R. J. Needs
P101-A	First-principles study of structural and dynamical properties of orthorhombic GaPO4 under hydrostatic pressure M. A. Padron-Brito, J.O Gonzalez-Lopez,, P. Rodriguez-Hernandez, <u>A. Munoz</u>
P101-B	Band structures and band gaps of dense hydrogen ---GW calculation Hitose Nagara, Takahiro Ishikawa, and Takao Kotani

Annex 4b: Final Budget

Bilan financier EHPRG 2014							
DEPENSES				RECETTES			
Libellés			Montants	Libellés			Montants
COMMUNICATION GENERALE			6 356,80 €				
Site internet + gestion mealing liste			1 500,00 €	Inscriptions congrès	Montant	202	87 580,00 €
Liste de diffusion à la charge de l'organisateur			offert				
Gestion de la plateforme d'inscription en ligne			2 000,00 €				
signalétique congrès - affiches diverses							
livre des actes			2 856,80 €				
				Subventions publiques			6 760,00 €
				UCBL			500,00 €
LOCATION LYON 3 la Manufacture			18 372,00 €	IML			1 000,00 €
Auditorium Malraux				FST			760,00 €
salles de plus de 60 places			18 372,00 €	ESF			2 500,00 €
Ménage				FRAMA			2 000,00 €
salon des symboles Nord							
MATERIEL - assistance technique			1 070,40 €				
ordinateurs + vidéo	5		offert				
assistance informatique	4	210,00 €	840,00 €	Sponsoring privé			9 350,00 €
location micros supplémentaire				Sanchez Technologies			1 400,00 €
location de panneaux poster (30 grilles)			offert UCBL	Depths of the earth company			2 000,00 €
Transport du matériel			230,40 €	Almax easylab			1 400,00 €
GESTION DES CONFERENCIERS (4)			5 287,52 €	Technodiamant			1 400,00 €
Hébergement 4 nuits Oddalys			1 807,35 €	SITEC			250,00 €
Transport Mr Girard Eric			65,44 €	BETSA			1 900,00 €
Mission Ma Yanming			1 800,00 €	Hp Systems			1 000,00 €
Mission McCAMMON Catherine			378,73 €				
Mission PARISE John			1 100,00 €				
fraix de gestion	4	34,00 €	136,00 €				
GESTION DES GRATUITS (35)			1 258,00 €				
fraix de gestion	37	34,00 €	1 258,00 €				
PERSONNELS			968,40 €				
1 Etudiants			88,40 €				
Informaticien forfait	4	220,00 €	880,00 €				
DIVERS			2 446,36 €				
Assurance MAIF	243	0,52 €	126,36 €				
Cotisation EHPRG	202	10,00 €	2 020,00 €				
Petites fournitures			300,00 €				
TOTAL FRAIS FIXES			35 759,48 €				
RESTAURATION SUR LA BASE DE 240			19 742,84 €				
pause matin et après-midi							
4 Déjeuners assis au CROUS			19 742,84 €				
PROGRAMME SOCIAL			23 529,88 €				
Musée des Beaux-Arts			308,00 €				
Visite Lyon			1 000,00 €				
Visite de Lyon en bus			935,00 €				
Dîner de Gala " Le Celsius"			14 506,88 €				
animation "la Farola Flamenca"			1 500,00 €				
Cocktail d'ouverture Odalys			2 850,00 €				
Pass TCL 4 jrs	243	10,00 €	2 430,00 €				
imprévus							
MALLETES CONGRESSISTES			486,00 €				
Sac à dos personnalisé			Fournis par BETSA				
bloc note + stylo			Fournis par Sanchez Technologies				
Badges lacet	243	2,00 €	486,00 €				
imprévus							
TOTAL FRAIS VARIABLES			43 758,72 €				
TOTAL FRAIS FIXES + VARIABLES			79 518,20 €				
FRAIS DE GESTION			24 171,80 €				
Frais de gestion Cellule Congrès 15%			15 553,50 €				
Frais de gestion UCBL			8 618,30 €				
TOTAL DEPENSES			103 690,00 €	TOTAL RECETTES			103 690,00 €

Annex 4c: Full list of speakers and participants

Shrikant	BHAT	DE	Allemagne
Attila	CANGI	DE	Allemagne
Leonid	DUBROVINSKY	DE	Allemagne
Jihaan	EBAD-ALLAH	DE	Allemagne
Jose a.	FLORES LIVAS	DE	Allemagne
Alexandra	FRIEDRICH	DE	Allemagne
Mydeen	KAMAL	DE	Allemagne
Christine	KUNTSCHER	DE	Allemagne
Anke	KÄHLER	DE	Allemagne
Christian	LATHE	DE	Allemagne
Catherine	MCCAMMON	DE	Allemagne
Sergiy	MEDVEDIEV	DE	Allemagne
Hans j.	MUELER	DE	Allemagne
Sergey	OVSYANNIKOV	DE	Allemagne
Dominik	PILAT	DE	Allemagne
Paul	SALMEN	DE	Allemagne
Uma maheswari	SANKARA SUBBIAH	DE	Allemagne
Julian	SCHULZE	DE	Allemagne
Natalia	SOLOPOVA	DE	Allemagne
Sergio	SPEZIALE	DE	Allemagne
Ronald	MILETICH	AT	Autriche
Rafael	ALENCAR	BR	Brésil
A. alberto	FERNANDES	BR	Brésil
Patricia	FERNANDES	BR	Brésil
Ana	SKURY	BR	Brésil
Altair	SORIA PEREIRA	BR	Brésil
Lixin	LIU	CN	Chine
Yanming	MA	CN	Chine
Liang	XU	CN	Chine
Mingguang	YAO	CN	Chine
Yongjae	LEE	KR	Corée du Sud
Miguel angel	ALARIO-FRANCO	ES	Espagne
Elena	DEL CORRO	ES	Espagne
Chantal	FERRER-ROCA	ES	Espagne
Jesus	GONZALEZ	ES	Espagne
Bérengère	GUIGNON	ES	Espagne
Jordi	IBANEZ	ES	Espagne
Fernando	IZQUIERDO RUIZ	ES	Espagne
Francisco javier	MANJÓN	ES	Espagne
Domingo	MARTINEZ-GARCIA	ES	Espagne
Virginia	MONTESGURO PADRÓN	ES	Espagne
Oscar r.	MONTORO	ES	Espagne
Angel	MORALES-GARCÍA	ES	Espagne
Andres	MUJICA	ES	Espagne

Alfonso	MUNOZ GONZALEZ	ES	Espagne
Robert	OLIVA	ES	Espagne
Catalin	POPESCU	ES	Espagne
Silvana	RADESCU	ES	Espagne
Fernando	RODRIGUEZ	ES	Espagne
Plácida	RODRIGUEZ-HERNANDEZ	ES	Espagne
Javier	SANCHEZ-BENITEZ	ES	Espagne
Juan angel	SANS TRESSERRAS	ES	Espagne
Alfredo	SEGURA	ES	Espagne
Mercedes	TARAVILLO	ES	Espagne
Garcia baonza	VALENTIN	ES	Espagne
Marit	PUUSEPP	EE	Estonie
Jay	BASS	US	Etats-Unis
Razvan	CARACAS	US	Etats-Unis
Robert	LIEBERMANN	US	Etats-Unis
Daniel	MAST	US	Etats-Unis
John	PARISE	US	Etats-Unis
Frederico	ALABARSE	FR	France
Sayed mohamed baqer	ALBAHRANI	FR	France
Muriel	ANDREANI	FR	France
Simon	AYRINHAC	FR	France
Victor	BALÉDENT	FR	France
Frederic	BEJINA	FR	France
Pierre	BOUVIER	FR	France
Eleonora	BOVE	FR	France
Yael	BRONSTEIN	FR	France
Hervé	CARDON	FR	France
Tiago	CERQUEIRA	FR	France
Kirill	CHEREDNICHENKO	FR	France
Antonio neves	DA SILVA	FR	France
Isabelle	DANIEL	FR	France
Frédéric	DATCHI	FR	France
Agnès	DEWAELE	FR	France
Maria ellen	DONNELLY	FR	France
Eliane	DUMAY	FR	France
Abstract	EHPRG2014	FR	France
Gaston	GARBARINO	FR	France
Valentina	GIORDANO	FR	France
Eric	GIRARD	FR	France
Eugene	GREGORYANZ	FR	France
Jeremy	GUIGNARD	FR	France
Jean-alexis	HERNANDEZ	FR	France
Olivier	ISNARD	FR	France
Jean-paul	ITIÉ	FR	France
Innokenty	KANTOR	FR	France

Stefan	KLOTZ	FR	France
Sylvie	LE FLOCH	FR	France
Claire	LEVELUT	FR	France
Cailong	LIU	FR	France
Denis	MACHON	FR	France
Jérémie	MARION	FR	France
Guillaume	MORARD	FR	France
Robson	MUNIZ	FR	France
Lucie	NATAF	FR	France
Sergey	NIKITIN	FR	France
Florent	OCCELLI	FR	France
Sakura	PASCARELLI	FR	France
Maria	PENS	FR	France
Jean-philippe	PERRILLAT	FR	France
Judith	PETERS	FR	France
David	PHILIPPON	FR	France
Vittoria	PISCHEDDA	FR	France
Antoni	PLANES	FR	France
Alain	POLIAN	FR	France
Arnaud	PROIETTI	FR	France
Torchio	RAFFAELLA	FR	France
Scheilla	RAMOS DA SILVA	FR	France
Umbertoluca	RANIERI	FR	France
Bruno	REYNARD	FR	France
Christian	ROUMESTAND	FR	France
Jerome	ROUQUETTE	FR	France
Daniela	RUSSO	FR	France
Alfonso	SAN MIGUEL	FR	France
Ninet	SANDRA	FR	France
Alexandra	SECLAMAN	FR	France
Aude	STOLZ	FR	France
Volodymyr	SVITLYK	FR	France
Nicolas	TERCé	FR	France
Abraao	TORRES DIAS	FR	France
Pierre	TOULEMONDE	FR	France
Coralie	WEIGEL	FR	France
Fabrice	WILHELM	FR	France
Dario	ALFE	GB	Grande-Bretagne
Craig	BULL	GB	Grande-Bretagne
Benjamin	COCHAIN	GB	Grande-Bretagne
David	DUNSTAN	GB	Grande-Bretagne
Juan	FALLAS	GB	Grande-Bretagne
Athina	FRANTZANA	GB	Grande-Bretagne
Mungo	FROST	GB	Grande-Bretagne
Malcolm	GUTHRIE	GB	Grande-Bretagne

Ross	HOWIE	GB	Grande-Bretagne
Konstantin	KAMENEV	GB	Grande-Bretagne
Ingo	LOA	GB	Grande-Bretagne
John	LOVEDAY	GB	Grande-Bretagne
James	POULTEN	GB	Grande-Bretagne
Ciprian	PRUTEANU	GB	Grande-Bretagne
Christopher	RIDLEY	GB	Grande-Bretagne
Andrei	SAPELKIN	GB	Grande-Bretagne
George	SERGHIOU	GB	Grande-Bretagne
Olga	SHEBANOVA	GB	Grande-Bretagne
Yiwei	SUN	GB	Grande-Bretagne
Heribert	WILHELM	GB	Grande-Bretagne
Yuanpeng	ZHANG	GB	Grande-Bretagne
John	ARVANITIDIS	GR	Grande-Bretagne
Dimitris	CHRISTOFILOS	GR	Grande-Bretagne
Gerasimos	KOUROUKLIS	GR	Grande-Bretagne
Efthymios	LIAROKAPIS	GR	Grande-Bretagne
Sotirios	VES	GR	Grande-Bretagne
Alba	CALVO GARCÍA	HU	Hongrie
Ildiko	KMECZ	HU	Hongrie
Csaba	NÉMETH	HU	Hongrie
Mahmoud	JAFARI	IR	Iran
Uri	ARGAMAN	IL	Israel
Moran	EMUNA	IL	Israel
Eran	GREENBERG	IL	Israel
Guy	MAKOV	IL	Israel
Gregory	ROZENBERG	IL	Israel
Eran	STERER	IL	Israel
Eyal	YAHIEL	IL	Israel
Rossella	ARLETTI	IT	Italie
Matteo	CEPPATELLI	IT	Italie
Marco	MERLINI	IT	Italie
Leonardo	PROPERZI	IT	Italie
Renato	PUCCI	IT	Italie
Mario	SANTORO	IT	Italie
Demetrio	SCELTA	IT	Italie
Katsutoshi	AOKI	JP	Japon
Hiroshi	FUKUI	JP	Japon
Ken-ichi	FUNAKOSHI	JP	Japon
Tetsuo	IRIFUNE	JP	Japon
Takahiro	ISHIKAWA	JP	Japon
Yuji	KAIHARA	JP	Japon
Kazuki	KOMATSU	JP	Japon
Tetsuji	KUME	JP	Japon
Keiji	KUNO	JP	Japon

Takahiro	MATSUOKA	JP	Japon
Masafumi	MATSUSHITA	JP	Japon
Hitose	NAGARA	JP	Japon
Satoshi	NAKANO	JP	Japon
Ayako	OHMURA	JP	Japon
Shinpei	YAMAMOTO	JP	Japon
Hitoshi	YUSA	JP	Japon
Roman	GAJDA	PL	Pologne
Andrzej	KATRUSIAK	PL	Pologne
Barbara	SOKOLOWSKA	PL	Pologne
Antonio	ALFAIA	PT	Portugal
Pavel	JAVORSKY	CZ	République Tchèque
Jaroslav	VALENTA	CZ	République Tchèque
Rasul	ARSLANOV	RU	Russie
Elena	BOLDYREVA	RU	Russie
Peter	DOROGOKUPETS	RU	Russie
Vadim	EFIMCHENKO	RU	Russie
Vladimir	GAPONTSEV	RU	Russie
Tatiana	GAPONTSEVA	RU	Russie
Igor	KOROBEYNIKOV	RU	Russie
Anna	LIKHACHEVA	RU	Russie
Konstantin	LITASOV	RU	Russie
Yuriy	LITVIN	RU	Russie
Nina	MELNIKOVA	RU	Russie
Akhmedbek	MOLLAEV	RU	Russie
Natalia	MOROZOVA	RU	Russie
Dmitry	NIKOLAEV	RU	Russie
Sergey	RASHCHENKO	RU	Russie
Fedor	SHAKHOV	RU	Russie
Tatyana	SOKOLOVA	RU	Russie
Galina	TIKHOMIROVA	RU	Russie
Yana	VOLKOVA	RU	Russie
Marian	MIHALIK	SK	Slovaquie
Matus	MIHALIK	SK	Slovaquie
Dusan	PLASIENKA	SK	Slovaquie
Igor	ABRIKOSOV	SE	Suède
Alexander	SOLDATOV	SE	Suède
Kristina	SPEKTOR	SE	Suède
Elodie	AMIGUET	CH	Suisse
Susannah	DORFMAN	CH	Suisse
Marc	SIEBER	CH	Suisse
Michaël	TRAN	CH	Suisse
Beat	ZEHNDER	CH	Suisse
Ergin murat	ALTUNER	TR	Turquie

