SORBONNE UNIVERSITÉ

PROGRAMME INSTITUTS ET INITIATIVES

Appel à projet – campagne 2021

Proposition de projet de recherche doctoral (PRD)

iMAT - Institut de Science des Matériaux

Intitulé du projet de recherche doctoral (PRD): Growth and Characterization of Bidimentionnal Pb Layers on Silicon Carbide Substrates

Directrice ou directeur de thèse porteuse ou porteur du projet (titulaire d'une HDR) :

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Unité de Recherche :
Intitulé : Institut des Nanosciences de Paris
Code *(ex. UMR xxxx)* : UMR 7588

École Doctorale de rattachement de l'équipe (future école doctorale de la doctorante ou du doctorant) : **ED397-Physique Chimie des Matériaux**

Doctorantes et doctorants actuellement encadrés par la directrice ou le directeur de thèse (préciser le nombre de doctorantes ou doctorants, leur année de 1e inscription et la quotité d'encadrement) : 1 doctorant, 1ère inscription en octobre 2018, encadré à 100%

Co-encadrante ou co-encadrant :

NOM : PREVOT Prénom : Geoffroy
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Unité de Recherche :
Intitulé : Institut des Nanosciences de Paris
Code *(ex. UMR xxxx)* : UMR 7588

École Doctorale de rattachement : **ED397-Physique Chimie des Matériaux**
Ou si ED non Alliance SU :

Doctorantes et doctorants actuellement encadrés par la directrice ou le directeur de thèse (préciser le nombre de doctorantes ou doctorants, leur année de 1e inscription et la quotité d'encadrement) : 2 doctorants encadrés à 50% chacun, 1ère inscription en octobre 2018

Co-encadrante ou co-encadrant :

NOM : Prénom :
Titre : Choisissez un élément : ou HDR ☐
e-mail :

Unité de Recherche :
Intitulé :
Code *(ex. UMR xxxx)* :

École Doctorale de rattachement : **Choisissez un élément :**
Ou si ED non Alliance SU :

Doctorantes et doctorants actuellement encadrés par la directrice ou le directeur de thèse (préciser le nombre de doctorantes ou doctorants, leur année de 1e inscription et la quotité d'encadrement) :

Cotutelle internationale : ☒ Non ☐ Oui, précisez Pays et Université :

Selon vous, ce projet est-il susceptible d'intéresser une autre Initiative ou un autre Institut ?
☒ Non ☐ Oui, précisez Choisissez l'institut ou l'initiative :

Description du projet de recherche doctoral ***(en français ou en anglais) :***

Ce texte sera diffusé en ligne : il ne doit pas excéder 3 pages et est écrit en interligne simple.

Détailler le contexte, l'objectif scientifique, la justification de l'approche scientifique ainsi que l'adéquation à l'initiative/l'Institut.

Le cas échéant, préciser le rôle de chaque encadrant ainsi que les compétences scientifiques apportées. Indiquer les publications/productions des encadrants en lien avec le projet.
Préciser le profil d'étudiant(e) recherché.

Opened by the discovery of graphene, an unexplored and broad road to new two-dimensional (2D) materials lies before us, and leads to a rich physics, which intimately connects fundamental research and technological applications. The possibilities offered by these 2D materials seem endless and have triggered intense and fruitful research in the community [1]. All these materials show a wide range of exceptional and exotic properties -in particular electronic properties- that can be used and combined to reach improved or even totally new performances.
Among all these properties, the Quantum Spin Hall (QSH) effect is one of the most promising in terms of applications. QSH materials are insulating in the bulk and exhibit characteristic helical edge states connecting valence and conduction bands. Furthermore, these edge states are oppositely spin-polarised and topologically protected from backscattering by time-reversal symmetry. Thus, these materials hold the promise of revolutionary spintronics devices with dissipation less spin current or the realization of Majorana bound states at the interface with superconductors [2].
Quantum Spin Hall effect was first predicted by Kane and Mele in graphene for which spin-orbit coupling (SOC) opens a gap at the Dirac points [3]. However, even at very low temperatures, the associated band gap is too small (in the order of 10-3 meV) to lead to detectable QSH effect in graphene. Moreover, up to now, despite numerous theoretical prediction on 2D QSH insulators, quantized conductance through QSH states have only been experimentally demonstrated in InAs/GaSb or HgTe/CdTe quantum wells [4] and Bi bilayers [5]. Again, due to a small bulk-gap in these systems, it is necessary to reach ultra-low temperatures to avoid contribution of bulk material to edge conduction by thermal excitation of carriers through the gap. And this represents a serious drawback for spintronics applications.

As the gap size depends, among others, on the SOC strength associated to the elements in the QSH material, it is natural to look for materials made of heavy elements. Following the example of graphene, other group-IV 2D materials, such as silicene, germanene or stanene have already been experimentally realized and explored. The associated gaps are higher than for graphene (around 200 meV), however, they remain too small for potential applications at reasonable temperatures.
On the other hand, Pb, which is the heaviest group-IV element, is predicted to show stable 2D phases exhibiting topological properties. However, the experimental investigations of this system are still scarce with, to our knowledge, only one evidence of the formation of so

called “plumbene” (2D Pb layer having a honeycomb structure) on a palladium substrate [6]. To go further and characterise the electronic properties of this Pb layer, it will be essential to transfer it from Pd to an insulating or semiconducting substrate, which can represent a major difficulty.
The ideal case would be to synthetize the 2D Pb layer directly on a semiconducting or isolating substrate. Several theoretical papers have recently proposed hexagonal silicon carbide (SiC) substrates as a good candidate for stabilization of a “plumbene” phase [7].

Our objective is thus the synthesis and characterisation of 2D Pb layers on semiconducting hexagonal silicon carbide substrates. No experimental studies on this system has been published yet and we would like to emphasize here that, beyond the only aspect of the growth of a QSH insulator layer, the Pb/SiC system is expected to show a rich physics as for Pb/Si or Pb/Ge with, for example, 2D superconductivity, Mott transitions or charge density waves evidenced so far.

The experimental techniques include STM/STS (at INSP in our teams), grazing incidence X-ray diffraction (GIXD, at synchrotron radiation (SR)), core-level / angle/spin resolved photoemission (XPS/ARPES, at SR and through our collaborations with Jean Lamour Institute in Nancy, Material and Surface Physics Laboratory in Cergy Pontoise, Solid States Physics laboratory in Orsay and Laboratory of Physics and Material studies at EPSCI). Density Functional Theory calculations can be also performed by our collaborators (Institut J. Lamour) to model growth and characterize the Pb/SiC interfaces.

In this context, an important part of this research project will deal with the synthesis of a plumbene layer by exploring the full phase diagram of Pb on SiC with STM. Atomic structure of the ordered phase will be determined by STM and GIXD, while information on the interaction of Pb atoms with the substrates will be given by XPS.

Calculations have proposed the possible formation of triangular phases of Pb on SiC(0001) surface [7]. Depending on the Pb coverage, different structures are expected such as a sparse triangular adatom structure for 1/3 of monolayer (ML), a honeycomb graphene-like structure (2/3 ML) or a dense triangular (1x1) structure. We would like to mention here that in reference [7] the authors only consider the adsorption of Pb atoms on a (1x1) bulk-like terminated SiC(0001) surface which can experimentally be obtained by ex-situ HF treatment. However, when prepared in-situ under ultra-high vacuum, SiC surfaces are known to exhibit several surface reconstructions depending on the Si/C ratio. This should further enrich the phase diagram of the Pb/SiC system. Among these reconstructions, the silicon-terminated SiC(0001) ($\sqrt{3}$x$\sqrt{3}$) looks like a good candidate to stabilize honeycomb Pb layers if we consider that, as on Si(111) surfaces, the Pb atoms will preferentially adsorb around the adatoms. To further promote the formation of honeycomb Pb structures at the expense of dense Pb layers, we can also think of saturating the adatoms dangling bond by interaction for example with oxygen atoms: it was shown that in the first step of oxidation of the SiC(0001) ($\sqrt{3}$x$\sqrt{3}$) surface, the overall atomic structure is preserved with oxygen atoms in the backbonds of the Si adatom and on its top [13].

Another aspect of this work will consist in the characterization of the electronic properties of the different phases of interest evidenced in the previous step. The triangular Pb phases predicted on SiC should exhibit cone-like features at K points originating mainly from px+py orbitals of the Pb atoms [7]. Furthermore, the intrinsic SOC of Pb should lead to a Zeeman-

like spin-splitting of the bulk bands. It is also predicted that the band originating from pz orbitals should exhibit Rashba-like spin polarization.
More particularly for plumbene, some theoretical studies predict it to be a trivial insulator [9]. But the substrate used for the 2D layer can play a major role in the stabilisation of the topological properties. For example, in the case of bismuthene on SiC surface, the substrate not only stabilizes the topological properties of the Bi film but also directly contribute to the large observed band gap by strong on-site SOC [10]. The evidence of eventual edge states characteristic of the QSH state, can be given by Scanning Tunnelling Spectroscopy through measurement of the differential conductivity at step edge for example. Systems of interest (not necessary QSH phase) can be further explored by ARPES (Synchrotron/LPEM ESPCI), spin-resolved ARPES (synchrotron/LPMS Cergy) or spin-resolved inverse photoemission experiments (LPS Orsay) which will provide a detailed picture of electronic properties of the 2D Pb layer.

[1] M. D'angelo and I. Matsuda, in "Monoatomic Two-Dimensional Layers", Elsevier, 2019
[2] L. Fu, C. L. Kane, Phys. Rev. Lett. 100, 096407 (2008).
[3] C. L. Kane & E. J. Mele, Phys. Rev. Lett. 95, 226801 (2005)
[4] B. Andrei Bernevig et al., Science 314, 1757 (2006)
[5] F. Yang et al., PRL109,016801 (2012)
[6] J. Yuhara et al., Adv. Mater. 31, 1901017 (2019)
[7] A. Visikovskiy et al., arXiv:1809.00829v1
[8] Y. Lu et al., Sci Rep 6, 21723 (2016)
[9] X.L. Yu et al., Phys. Rev. B 95, 125113 (2017)
[10] F. Reis et al., Science 357, 287 (2017)
[11] H. Zhao et al., Sci Rep. 6, 20152 (2016)
[12] M. D'angelo, Journal of Physics D, 51, 433001 (2018)
[13] W. Voegeli et al., Surf. Science 604, 1713 (2010)

Rôle de chaque encadrant / compétences scientifiques apportées
G. Prévot and M. D'angelo have both a long-standing expertise in the growth of monoatomic 2D layers and their characterization with STM. The project will benefit from the recent acquisition of a commercial Variable-Temperature STM (M. D'angelo's team), which is an easy handling setup particularly suitable for the search for Pb phases on SiC substrates. These experiments will be performed under the supervision of both co-proposers. In addition, G. Prévot, who is an expert of grazing incidence X-ray diffraction, will be leading the experiments for the determination of the atomic structure of the Pb phases. On the other hand, M. D'angelo, who is specialist of core-level and angle-resolved photoemission will supervise the experiments related to the determination of the electronic properties of the Pb layers.

Publications des encadrants en lien avec le sujet
- M. D'angelo and I. Matsuda, "Monoatomic Two-Dimensional Layers", Elsevier, 2019 (book chapter)
- M. Cameau et al., Phys. Rev. Materials 3, 044004 (2019)
- M. D'angelo, Journal of Physics D, 51, 433001, (2018) (review article)
- C.C. Lee et al., Physical Review B 97 (7), 075430 (2018)
- C. Tresca et al., Physical Review Letters 120, 196402 (2018)

- M. D'Angelo et al., Phys. Rev. Let. 108, 116802 (2012)
- P. Soukiassian, et al., Nature Com. 4, 2800 (2013)
- M. D'angelo et al., Phys. Rev. B 79, 035318 (2009)
- V. Derycke et al., Nature Mat. 2, 253 (2003)
- G. Prévot et al., Appl. Phys. Lett. 105 (2014) 213106
- G. Prévot et al., Phys. Rev. Lett. 117 (2016) 276102
- A. Curcella et al., 2D Materials 4 (2017) 025067
- A. Curcella et al., Nanoscale 10 (2018) 2291
- W. Peng et al., ACS Nano 12 (2018) 4754
- K. Zhang et al., Phys. Rev. B 102 (2020) 125418

Profil recherché

The candidate must have a good knowledge of basic general physics. A specialisation in material and surface sciences will be appreciated but is not compulsory. On the other hand, a pronounced taste for experimental physics is needed.

Fichier envoyer simultanément par e-mail à l'ED de rattachement et au programme :
cd_instituts_et_initiatives@listes.upmc.fr avant le 20 février.